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Compound 1a

X-RAY DIFFRACTION STUDY

Data collection, crystal, and refinement parameters are collected in Table 1. The unit cell parameters were obtained from the least-squares fit of 25 reflections (with θ between 10° and 20°). Data were collected with the ω-2θ scan technique and a variable scan rate, with a maximum scan time of 60 s per reflection. The final drift correction factors were between 0.99 and 1.06. On all reflections, profile analysis[2,4] was performed. Lorentz and polarization corrections were applied and the data were reduced to $|F_o|$ values.

The structure was solved by DIRDIF[1] (Patterson methods and phase expansion). Isotropic least-squares refinement using SHELX76[6,9] converged to R = 0.121. At this stage an empirical absorption correction was applied using DIFABS[10].

Hydrogen atoms were geometrically placed. During the final stages of the refinement, the positional parameters and the anisotropic thermal parameters of the non-H atoms were refined. The geometrically placed hydrogen atoms were isotropically refined with a common thermal parameter, riding on their parent atoms.

Finally, a full-matrix least-squares refinement on F^2 was made using SHELXL93[7]. The function minimized was $[\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w (F_o^2)^2]^{1/2}$, $w = 1 / [\sigma^2 (F_o^2) + (0.1106 * P)^2]$ where $P = (\text{Max} (F_o^2, 0) + 2 * F_c^2) / 3$ with $\sigma^2 (F_o^2)$ from counting statistics. The maximum shift to e.s.d. ratio in the last full-matrix least-squares cycle was 0.001. The CH_2Cl_2 solvent molecule was affected of strong structural disorder. The Cl-atoms were isotropically refined, and one of them, (Cl(2)), was found in two disordered positions (occupation factors = 0.57(1) and 0.43(1)). Its hydrogen atoms were geometrically placed but two different positions were refined, one for each Cl(2) position. The final difference Fourier map showed no peaks higher than 0.81 eÅ^{-3}, nor deeper than -1.01 eÅ^{-3}. Atomic scattering factors were taken from International Tables for X-Ray Crystallography (1974)[3]. Geometrical calculations were made with PARST[5]. The crystallographic plots were made with EUCLID[8]. All calculations were made at the University of Oviedo on the Scientific Computer Center and X-Ray group VAX-computers. This work was partially supported by DGICYT (PB93 - 0330). Javier Borge thanks to the Ministerio de Educación y Ciencia (Spain) for a fellowship.

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Table 1. Crystal data and structure refinement parameters. L2147-3

Identification code	VC12
Empirical formula	$[C_{60}H_{47}P_2Ru^+][PF_6^-]\cdot CH_2Cl_2$
Formula weight	1160.88
Temperature	293 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P $2_1/c$
Unit cell dimensions	a = 13.339(3) Å α = 90° b = 19.67(2) Å β = 99.88(4)° c = 20.82(1) Å γ = 90°
Volume	5382(5) Å^3
Z	4
Density (calculated)	1.433 Mg/m^3
Absorption coefficient	0.540 mm^{-1}
F(000)	2368
Crystal size	0.30 x 0.26 x 0.23 mm
Theta range for data collection	1.43° to 24.97°
Index ranges	$0 \le h \le 15$ $0 \le k \le 23$ $-24 \le l \le 24$
Reflections collected	10038
Independent reflections	9443 [R_{int} = 0.054]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9393 / 4 / 655
Goodness-of-fit on F^2	0.943
Final R indices [I>2σ(I)]	R1 = 0.0548, wR2 = 0.1445
R indices (all data)	R1 = 0.1228, wR2 = 0.1720
Largest diff. peak and hole	0.811 and -1.005 eÅ^{-3}

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	3163(1)	917(1)	1503(1)	33(1)
P(1)	2428(1)	1639(1)	2173(1)	36(1)
P(2)	4619(1)	636(1)	2268(1)	35(1)
C(11)	1033(3)	1572(2)	2068(3)	40(1)
C(12)	529(4)	1766(3)	2574(3)	58(2)
C(13)	-513(5)	1758(4)	2491(4)	75(2)
C(14)	-1075(4)	1545(4)	1898(4)	79(2)
C(15)	-580(4)	1363(4)	1408(4)	84(2)
C(16)	480(4)	1371(3)	1489(3)	63(2)
C(21)	2775(4)	1612(3)	3065(2)	41(1)
C(22)	2626(4)	1004(3)	3367(3)	55(1)
C(23)	2824(6)	957(4)	4047(4)	77(2)
C(24)	3192(5)	1511(5)	4409(3)	76(2)
C(25)	3345(4)	2128(4)	4114(3)	67(2)
C(26)	3139(4)	2175(3)	3436(3)	53(1)
C(31)	2614(4)	2530(3)	1984(3)	43(1)
C(32)	3603(4)	2781(3)	2015(3)	47(1)
C(33)	3765(5)	3447(3)	1876(3)	65(2)
C(34)	2958(6)	3877(3)	1702(5)	92(3)
C(35)	1996(6)	3653(4)	1676(5)	116(4)
C(36)	1806(4)	2977(3)	1801(4)	73(2)
C(41)	5497(4)	74(3)	1923(3)	43(1)
C(42)	6537(4)	162(3)	2040(3)	61(2)
C(43)	7140(5)	-294(4)	1763(4)	81(2)
C(44)	6723(6)	-818(4)	1387(4)	76(2)
C(45)	5698(5)	-921(3)	1293(3)	70(2)
C(46)	5072(5)	-488(3)	1562(3)	55(1)
C(51)	5379(3)	1392(3)	2527(2)	38(1)
C(52)	5915(4)	1708(3)	2092(3)	45(1)
C(53)	6414(4)	2315(3)	2239(3)	54(1)
C(54)	6386(4)	2619(3)	2834(3)	64(2)
C(55)	5843(5)	2337(3)	3268(3)	60(2)
C(56)	5345(4)	1725(3)	3119(3)	47(1)
C(61)	4542(3)	154(3)	3013(3)	41(1)
C(62)	3782(4)	-340(3)	3012(3)	50(1)
C(63)	3753(5)	-738(3)	3552(3)	62(2)
C(64)	4454(5)	-658(3)	4096(3)	64(2)
C(65)	5218(5)	-194(4)	4115(3)	69(2)
C(66)	5273(4)	205(3)	3568(3)	54(2)
C(70)	3348(4)	582(3)	439(2)	44(1)
C(71)	4168(4)	1024(3)	744(2)	52(1)
C(72)	3764(4)	1668(3)	837(3)	49(1)
C(73)	2706(4)	1620(3)	663(2)	48(1)
C(74)	2435(4)	963(3)	388(2)	46(1)
C(75)	1506(4)	668(3)	84(3)	49(1)
C(76)	1528(5)	21(3)	-151(3)	65(2)
C(77)	2427(5)	-350(3)	-89(3)	67(2)
C(78)	3321(5)	-84(3)	196(3)	60(2)
C(1)	2317(3)	217(2)	1711(3)	40(1)
C(2)	1690(4)	-259(3)	1729(3)	54(1)
C(3)	1069(4)	-754(3)	1883(3)	54(2)
C(81)	848(4)	-773(3)	2551(3)	61(2)
C(82)	612(6)	-200(5)	2864(4)	93(3)
C(83)	461(9)	-232(7)	3495(7)	146(5)
C(84)	586(9)	-807(9)	3832(6)	153(7)
C(85)	824(6)	-1390(7)	3556(5)	118(4)
C(86)	947(5)	-1390(4)	2902(4)	86(2)
C(91)	617(4)	-1273(3)	1409(3)	54(2)
C(92)	1101(5)	-1480(3)	908(4)	71(2)
C(93)	672(6)	-1965(4)	461(4)	84(2)
C(94)	-250(6)	-2244(4)	522(4)	88(2)
C(95)	-749(5)	-2046(4)	1000(4)	78(2)

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor. (Cont.).

	x	y	z	U_{eq}
C(96)	-325(4)	-1568(3)	1452(3)	66(2)
P(3)	6408(1)	2591(1)	5246(1)	57(1)
F(1)	5702(4)	2333(2)	5735(2)	100(1)
F(2)	5453(4)	2952(3)	4844(3)	123(2)
F(3)	6652(4)	3239(3)	5688(2)	122(2)
F(4)	6113(5)	1945(2)	4801(2)	122(2)
F(5)	7044(4)	2861(3)	4742(2)	144(2)
F(6)	7270(5)	2185(5)	5652(3)	198(4)
Cl(1)[1]	1953(4)	5200(3)	428(2)	209(2)
Cl(2)[2]	1958(6)	6075(4)	1394(4)	185(4)
Cl(2')[3]	672(10)	6235(6)	649(6)	235(7)
C(900)	1962(12)	6077(7)	596(7)	357(18)

[1] U_{iso} x 10^3
[2] U_{iso} x 10^3, Occupation factor = 0.57(1)
[3] U_{iso} x 10^3, Occupation factor = 0.43(1)

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Table 3. Bond lengths [Å].

Ru(1)-C(1)	1.878(5)
Ru(1)-C(73)	2.230(5)
Ru(1)-C(71)	2.251(5)
Ru(1)-C(72)	2.264(5)
Ru(1)-P(1)	2.321(2)
Ru(1)-P(2)	2.358(2)
Ru(1)-C(74)	2.359(5)
Ru(1)-C(70)	2.364(5)
P(1)-C(31)	1.822(5)
P(1)-C(21)	1.837(5)
P(1)-C(11)	1.842(5)
P(2)-C(51)	1.829(5)
P(2)-C(61)	1.835(5)
P(2)-C(41)	1.844(5)
C(11)-C(16)	1.359(8)
C(11)-C(12)	1.396(7)
C(12)-C(13)	1.371(8)
C(12)-H(12)	0.93
C(13)-C(14)	1.39(1)
C(13)-H(13)	0.93
C(14)-C(15)	1.357(9)
C(14)-H(14)	0.93
C(15)-C(16)	1.395(8)
C(15)-H(15)	0.93
C(16)-H(16)	0.93
C(21)-C(22)	1.380(8)
C(21)-C(26)	1.390(7)
C(22)-C(23)	1.397(9)
C(22)-H(22)	0.93
C(23)-C(24)	1.37(1)
C(23)-H(23)	0.93
C(24)-C(25)	1.39(1)
C(24)-H(24)	0.93
C(25)-C(26)	1.394(8)
C(25)-H(25)	0.93
C(26)-H(26)	0.93
C(31)-C(36)	1.393(7)
C(31)-C(32)	1.400(7)
C(32)-C(33)	1.368(8)
C(32)-H(32)	0.93
C(33)-C(34)	1.369(9)
C(33)-H(33)	0.93
C(34)-C(35)	1.35(1)
C(34)-H(34)	0.93
C(35)-C(36)	1.388(9)
C(35)-H(35)	0.93
C(36)-H(36)	0.93
C(41)-C(42)	1.379(7)
C(41)-C(46)	1.401(8)
C(42)-C(43)	1.393(8)
C(42)-H(42)	0.93
C(43)-C(44)	1.35(1)
C(43)-H(43)	0.93
C(44)-C(45)	1.363(9)
C(44)-H(44)	0.93
C(45)-C(46)	1.376(8)
C(45)-H(45)	0.93
C(46)-H(46)	0.93
C(51)-C(52)	1.392(7)
C(51)-C(56)	1.404(7)
C(52)-C(53)	1.376(7)
C(52)-H(52)	0.93
C(53)-C(54)	1.382(9)
C(53)-H(53)	0.93
C(54)-C(55)	1.367(9)
C(54)-H(54)	0.93
C(55)-C(56)	1.384(8)

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Table 3. Bond lengths [Å]. (Cont.).

C(55)-H(55)	0.93
C(56)-H(56)	0.93
C(61)-C(66)	1.381(7)
C(61)-C(62)	1.404(7)
C(62)-C(63)	1.375(8)
C(62)-H(62)	0.93
C(63)-C(64)	1.349(9)
C(63)-H(63)	0.93
C(64)-C(65)	1.363(9)
C(64)-H(64)	0.93
C(65)-C(66)	1.396(8)
C(65)-H(65)	0.93
C(66)-H(66)	0.93
C(70)-C(78)	1.403(8)
C(70)-C(74)	1.418(7)
C(70)-C(71)	1.455(7)
C(71)-C(72)	1.404(8)
C(71)-H(71)	0.93
C(72)-C(73)	1.399(7)
C(72)-H(72)	0.93
C(73)-C(74)	1.433(8)
C(73)-H(73)	0.93
C(74)-C(75)	1.417(7)
C(75)-C(76)	1.365(8)
C(75)-H(75)	0.93
C(76)-C(77)	1.391(9)
C(76)-H(76)	0.93
C(77)-C(78)	1.344(8)
C(77)-H(77)	0.93
C(78)-H(78)	0.93
C(1)-C(2)	1.260(7)
C(2)-C(3)	1.353(7)
C(3)-C(81)	1.469(9)
C(3)-C(91)	1.475(8)
C(81)-C(82)	1.36(1)
C(81)-C(86)	1.413(9)
C(82)-C(83)	1.36(1)
C(82)-H(82)	0.93
C(83)-C(84)	1.33(2)
C(83)-H(83)	0.93
C(84)-C(85)	1.34(2)
C(84)-H(84)	0.93
C(85)-C(86)	1.40(1)
C(85)-H(85)	0.93
C(86)-H(86)	0.93
C(91)-C(92)	1.379(9)
C(91)-C(96)	1.402(7)
C(92)-C(93)	1.39(1)
C(92)-H(92)	0.93
C(93)-C(94)	1.37(1)
C(93)-H(93)	0.93
C(94)-C(95)	1.35(1)
C(94)-H(94)	0.93
C(95)-C(96)	1.38(1)
C(95)-H(95)	0.93
C(96)-H(96)	0.93
P(3)-F(6)	1.530(5)
P(3)-F(5)	1.552(4)
P(3)-F(2)	1.570(5)
P(3)-F(3)	1.573(5)
P(3)-F(4)	1.582(5)
P(3)-F(1)	1.584(4)
Cl(1)-C(900)	1.76(1)
C(900)-Cl(2)	1.66(1)
C(900)-Cl(2')	1.77(2)

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Table 3. Bond lengths [Å]. (Cont.).

C(900)-H(99A)[1]	0.97
C(900)-H(99B)[1]	0.97
C(900)-H(99C)[2]	0.97
C(900)-H(99D)[2]	0.97

[1] Occupation factor = 0.57(1)
[2] Occupation factor = 0.43(1)

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Table 4. Bond angles [°].

C(1)-Ru(1)-C(73)	122.8(2)
C(1)-Ru(1)-C(71)	133.2(2)
C(73)-Ru(1)-C(71)	60.5(2)
C(1)-Ru(1)-C(72)	155.5(2)
C(73)-Ru(1)-C(72)	36.3(2)
C(71)-Ru(1)-C(72)	36.2(2)
C(1)-Ru(1)-P(1)	88.7(2)
C(73)-Ru(1)-P(1)	90.3(2)
C(71)-Ru(1)-P(1)	136.8(2)
C(72)-Ru(1)-P(1)	101.5(2)
C(1)-Ru(1)-P(2)	97.4(2)
C(73)-Ru(1)-P(2)	139.3(2)
C(71)-Ru(1)-P(2)	88.6(2)
C(72)-Ru(1)-P(2)	103.3(2)
P(1)-Ru(1)-P(2)	96.95(5)
C(1)-Ru(1)-C(74)	95.4(2)
C(73)-Ru(1)-C(74)	36.3(2)
C(71)-Ru(1)-C(74)	60.0(2)
C(72)-Ru(1)-C(74)	60.1(2)
P(1)-Ru(1)-C(74)	115.0(1)
P(2)-Ru(1)-C(74)	145.7(1)
C(1)-Ru(1)-C(70)	100.1(2)
C(73)-Ru(1)-C(70)	59.8(2)
C(71)-Ru(1)-C(70)	36.6(2)
C(72)-Ru(1)-C(70)	60.2(2)
P(1)-Ru(1)-C(70)	148.9(1)
P(2)-Ru(1)-C(70)	111.2(1)
C(74)-Ru(1)-C(70)	34.9(2)
C(31)-P(1)-C(21)	103.0(2)
C(31)-P(1)-C(11)	102.4(2)
C(21)-P(1)-C(11)	101.0(2)
C(31)-P(1)-Ru(1)	111.9(2)
C(21)-P(1)-Ru(1)	122.1(2)
C(11)-P(1)-Ru(1)	114.1(2)
C(51)-P(2)-C(61)	106.3(2)
C(51)-P(2)-C(41)	104.2(2)
C(61)-P(2)-C(41)	98.7(2)
C(51)-P(2)-Ru(1)	111.0(2)
C(61)-P(2)-Ru(1)	122.2(2)
C(41)-P(2)-Ru(1)	112.4(2)
C(16)-C(11)-C(12)	119.4(5)
C(16)-C(11)-P(1)	120.5(4)
C(12)-C(11)-P(1)	119.9(4)
C(13)-C(12)-C(11)	120.7(6)
C(13)-C(12)-H(12)	119.7(4)
C(11)-C(12)-H(12)	119.7(3)
C(12)-C(13)-C(14)	119.7(6)
C(12)-C(13)-H(13)	120.2(4)
C(14)-C(13)-H(13)	120.2(4)
C(15)-C(14)-C(13)	119.3(5)
C(15)-C(14)-H(14)	120.4(4)
C(13)-C(14)-H(14)	120.4(4)
C(14)-C(15)-C(16)	121.3(6)
C(14)-C(15)-H(15)	119.4(4)
C(16)-C(15)-H(15)	119.4(4)
C(11)-C(16)-C(15)	119.7(6)
C(11)-C(16)-H(16)	120.2(3)
C(15)-C(16)-H(16)	120.2(4)
C(22)-C(21)-C(26)	120.1(5)
C(22)-C(21)-P(1)	117.1(4)
C(26)-C(21)-P(1)	122.8(4)
C(21)-C(22)-C(23)	120.1(6)
C(21)-C(22)-H(22)	119.9(3)
C(23)-C(22)-H(22)	119.9(4)
C(24)-C(23)-C(22)	119.5(7)
C(24)-C(23)-H(23)	120.2(5)
C(22)-C(23)-H(23)	120.2(4)

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Table 4. Bond angles [°]. (Cont.).

C(23)-C(24)-C(25)	121.2(6)
C(23)-C(24)-H(24)	119.4(4)
C(25)-C(24)-H(24)	119.4(4)
C(24)-C(25)-C(26)	119.1(6)
C(24)-C(25)-H(25)	120.4(4)
C(26)-C(25)-H(25)	120.4(4)
C(21)-C(26)-C(25)	119.9(6)
C(21)-C(26)-H(26)	120.0(3)
C(25)-C(26)-H(26)	120.0(4)
C(36)-C(31)-C(32)	117.9(5)
C(36)-C(31)-P(1)	122.7(4)
C(32)-C(31)-P(1)	119.4(4)
C(33)-C(32)-C(31)	120.7(5)
C(33)-C(32)-H(32)	119.6(3)
C(31)-C(32)-H(32)	119.6(3)
C(32)-C(33)-C(34)	120.2(6)
C(32)-C(33)-H(33)	119.9(3)
C(34)-C(33)-H(33)	119.9(4)
C(35)-C(34)-C(33)	120.5(6)
C(35)-C(34)-H(34)	119.7(4)
C(33)-C(34)-H(34)	119.7(4)
C(34)-C(35)-C(36)	120.6(6)
C(34)-C(35)-H(35)	119.7(4)
C(36)-C(35)-H(35)	119.7(4)
C(35)-C(36)-C(31)	120.0(6)
C(35)-C(36)-H(36)	120.0(4)
C(31)-C(36)-H(36)	120.0(3)
C(42)-C(41)-C(46)	119.7(5)
C(42)-C(41)-P(2)	122.9(4)
C(46)-C(41)-P(2)	117.3(4)
C(41)-C(42)-C(43)	118.7(6)
C(41)-C(42)-H(42)	120.6(3)
C(43)-C(42)-H(42)	120.6(4)
C(44)-C(43)-C(42)	121.4(6)
C(44)-C(43)-H(43)	119.3(4)
C(42)-C(43)-H(43)	119.3(4)
C(43)-C(44)-C(45)	119.9(6)
C(43)-C(44)-H(44)	120.1(4)
C(45)-C(44)-H(44)	120.1(4)
C(44)-C(45)-C(46)	120.9(6)
C(44)-C(45)-H(45)	119.6(4)
C(46)-C(45)-H(45)	119.6(4)
C(45)-C(46)-C(41)	119.3(6)
C(45)-C(46)-H(46)	120.4(4)
C(41)-C(46)-H(46)	120.4(3)
C(52)-C(51)-C(56)	117.4(5)
C(52)-C(51)-P(2)	119.5(4)
C(56)-C(51)-P(2)	122.6(4)
C(53)-C(52)-C(51)	121.8(5)
C(53)-C(52)-H(52)	119.1(3)
C(51)-C(52)-H(52)	119.1(3)
C(52)-C(53)-C(54)	119.1(6)
C(52)-C(53)-H(53)	120.5(3)
C(54)-C(53)-H(53)	120.5(4)
C(55)-C(54)-C(53)	121.1(5)
C(55)-C(54)-H(54)	119.5(4)
C(53)-C(54)-H(54)	119.5(4)
C(54)-C(55)-C(56)	119.6(6)
C(54)-C(55)-H(55)	120.2(4)
C(56)-C(55)-H(55)	120.2(4)
C(55)-C(56)-C(51)	121.0(5)
C(55)-C(56)-H(56)	119.5(4)
C(51)-C(56)-H(56)	119.5(3)
C(66)-C(61)-C(62)	117.2(5)
C(66)-C(61)-P(2)	122.3(4)
C(62)-C(61)-P(2)	120.1(4)
C(63)-C(62)-C(61)	121.0(5)

Table 4. Bond angles [°]. (Cont.).

C(63)-C(62)-H(62)	119.5(4)
C(61)-C(62)-H(62)	119.5(3)
C(64)-C(63)-C(62)	120.4(6)
C(64)-C(63)-H(63)	119.8(4)
C(62)-C(63)-H(63)	119.8(4)
C(63)-C(64)-C(65)	120.6(6)
C(63)-C(64)-H(64)	119.7(4)
C(65)-C(64)-H(64)	119.7(4)
C(64)-C(65)-C(66)	119.8(6)
C(64)-C(65)-H(65)	120.1(4)
C(66)-C(65)-H(65)	120.1(4)
C(61)-C(66)-C(65)	120.9(6)
C(61)-C(66)-H(66)	119.6(3)
C(65)-C(66)-H(66)	119.6(4)
C(78)-C(70)-C(74)	119.9(5)
C(78)-C(70)-C(71)	133.3(5)
C(74)-C(70)-C(71)	106.8(5)
C(78)-C(70)-Ru(1)	126.6(4)
C(74)-C(70)-Ru(1)	72.3(3)
C(71)-C(70)-Ru(1)	67.4(3)
C(72)-C(71)-C(70)	108.7(5)
C(72)-C(71)-Ru(1)	72.4(3)
C(70)-C(71)-Ru(1)	75.9(3)
C(72)-C(71)-H(71)	125.6(3)
C(70)-C(71)-H(71)	125.6(3)
Ru(1)-C(71)-H(71)	117.9(2)
C(73)-C(72)-C(71)	107.3(5)
C(73)-C(72)-Ru(1)	70.5(3)
C(71)-C(72)-Ru(1)	71.4(3)
C(73)-C(72)-H(72)	126.4(3)
C(71)-C(72)-H(72)	126.4(3)
Ru(1)-C(72)-H(72)	123.4(2)
C(72)-C(73)-C(74)	109.8(5)
C(72)-C(73)-Ru(1)	73.2(3)
C(74)-C(73)-Ru(1)	76.8(3)
C(72)-C(73)-H(73)	125.1(3)
C(74)-C(73)-H(73)	125.1(3)
Ru(1)-C(73)-H(73)	116.8(2)
C(75)-C(74)-C(70)	119.4(5)
C(75)-C(74)-C(73)	133.6(5)
C(70)-C(74)-C(73)	107.0(4)
C(75)-C(74)-Ru(1)	127.1(4)
C(70)-C(74)-Ru(1)	72.7(3)
C(73)-C(74)-Ru(1)	67.0(3)
C(76)-C(75)-C(74)	118.1(5)
C(76)-C(75)-H(75)	121.0(3)
C(74)-C(75)-H(75)	121.0(3)
C(75)-C(76)-C(77)	121.9(6)
C(75)-C(76)-H(76)	119.0(3)
C(77)-C(76)-H(76)	119.0(4)
C(78)-C(77)-C(76)	121.4(6)
C(78)-C(77)-H(77)	119.3(4)
C(76)-C(77)-H(77)	119.3(4)
C(77)-C(78)-C(70)	119.3(6)
C(77)-C(78)-H(78)	120.4(4)
C(70)-C(78)-H(78)	120.4(3)
C(2)-C(1)-Ru(1)	168.5(5)
C(1)-C(2)-C(3)	168.2(7)
C(2)-C(3)-C(81)	118.2(6)
C(2)-C(3)-C(91)	122.4(6)
C(81)-C(3)-C(91)	119.4(5)
C(82)-C(81)-C(86)	118.1(7)
C(82)-C(81)-C(3)	122.1(6)
C(86)-C(81)-C(3)	119.6(7)
C(81)-C(82)-C(83)	120.(1)
C(81)-C(82)-H(82)	119.8(5)
C(83)-C(82)-H(82)	119.8(8)

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Table 4. Bond angles [°]. (Cont.).

C(84)-C(83)-C(82)	121.(1)
C(84)-C(83)-H(83)	119.3(9)
C(82)-C(83)-H(83)	119.3(8)
C(83)-C(84)-C(85)	121.(1)
C(83)-C(84)-H(84)	119.4(9)
C(85)-C(84)-H(84)	119.4(9)
C(84)-C(85)-C(86)	119.(1)
C(84)-C(85)-H(85)	120.3(9)
C(86)-C(85)-H(85)	120.3(7)
C(85)-C(86)-C(81)	119.2(9)
C(85)-C(86)-H(86)	120.4(7)
C(81)-C(86)-H(86)	120.4(5)
C(92)-C(91)-C(96)	117.8(6)
C(92)-C(91)-C(3)	121.4(5)
C(96)-C(91)-C(3)	120.7(6)
C(91)-C(92)-C(93)	121.3(6)
C(91)-C(92)-H(92)	119.3(4)
C(93)-C(92)-H(92)	119.3(4)
C(94)-C(93)-C(92)	119.0(8)
C(94)-C(93)-H(93)	120.5(5)
C(92)-C(93)-H(93)	120.5(4)
C(95)-C(94)-C(93)	121.2(8)
C(95)-C(94)-H(94)	119.4(4)
C(93)-C(94)-H(94)	119.4(5)
C(94)-C(95)-C(96)	120.3(7)
C(94)-C(95)-H(95)	119.9(4)
C(96)-C(95)-H(95)	119.9(4)
C(95)-C(96)-C(91)	120.4(7)
C(95)-C(96)-H(96)	119.8(4)
C(91)-C(96)-H(96)	119.8(4)
F(6)-P(3)-F(5)	96.1(4)
F(6)-P(3)-F(2)	174.5(4)
F(5)-P(3)-F(2)	88.4(4)
F(6)-P(3)-F(3)	92.3(4)
F(5)-P(3)-F(3)	92.0(3)
F(2)-P(3)-F(3)	90.7(3)
F(6)-P(3)-F(4)	89.6(4)
F(5)-P(3)-F(4)	89.3(3)
F(2)-P(3)-F(4)	87.4(3)
F(3)-P(3)-F(4)	177.6(3)
F(6)-P(3)-F(1)	87.2(4)
F(5)-P(3)-F(1)	176.7(3)
F(2)-P(3)-F(1)	88.3(3)
F(3)-P(3)-F(1)	88.3(2)
F(4)-P(3)-F(1)	90.3(3)
Cl(2)-C(900)-Cl(1)	101.3(7)
Cl(1)-C(900)-Cl(2')	102.2(7)
Cl(2)-C(900)-H(99A)	111.5(5)
Cl(1)-C(900)-H(99A)	111.5(6)
Cl(2)-C(900)-H(99B)	111.5(6)
Cl(1)-C(900)-H(99B)	111.5(5)
H(99A)-C(900)-H(99B)	109.3
Cl(1)-C(900)-H(99C)	111.3(5)
Cl(2')-C(900)-H(99C)	111.3(6)
Cl(1)-C(900)-H(99D)	111.3(5)
Cl(2')-C(900)-H(99D)	111.3(6)
H(99C)-C(900)-H(99D)	109.2

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Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}].

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{13}
Ru(1)	32(1)	33(1)	34(1)	-1(1)	6(1)	-4(1)
P(1)	33(1)	34(1)	41(1)	-4(1)	5(1)	-1(1)
P(2)	34(1)	36(1)	37(1)	0(1)	8(1)	0(1)
C(11)	35(2)	31(3)	52(3)	-4(2)	5(2)	-1(2)
C(12)	47(3)	64(4)	64(4)	-11(3)	12(3)	2(3)
C(13)	49(3)	91(5)	91(5)	-14(4)	29(4)	10(3)
C(14)	28(3)	83(5)	125(7)	-11(5)	12(4)	3(3)
C(15)	40(3)	108(6)	96(6)	-45(5)	-8(3)	-3(3)
C(16)	38(3)	82(5)	67(4)	-29(4)	6(3)	-1(3)
C(21)	36(2)	50(3)	37(3)	-7(2)	6(2)	0(2)
C(22)	59(3)	62(4)	44(3)	0(3)	12(3)	8(3)
C(23)	87(5)	76(5)	71(5)	15(4)	23(4)	18(4)
C(24)	73(4)	114(7)	38(4)	-1(4)	5(3)	21(4)
C(25)	53(3)	97(5)	50(4)	-32(4)	4(3)	0(3)
C(26)	39(3)	64(4)	55(4)	-15(3)	10(3)	-1(3)
C(31)	41(3)	35(3)	52(3)	-4(2)	3(2)	2(2)
C(32)	38(3)	44(3)	56(3)	6(3)	-1(2)	-3(2)
C(33)	58(3)	46(4)	89(5)	4(3)	4(3)	-14(3)
C(34)	79(5)	35(3)	157(8)	17(4)	8(5)	-6(3)
C(35)	67(5)	43(4)	228(12)	27(6)	3(6)	17(3)
C(36)	44(3)	48(4)	124(6)	11(4)	0(3)	0(3)
C(41)	50(3)	38(3)	45(3)	4(2)	19(2)	9(2)
C(42)	42(3)	56(4)	87(5)	-11(3)	16(3)	5(3)
C(43)	54(4)	76(5)	120(7)	-7(5)	33(4)	21(3)
C(44)	84(5)	66(5)	86(5)	-11(4)	36(4)	21(4)
C(45)	88(5)	53(4)	68(4)	-18(3)	9(4)	19(4)
C(46)	62(3)	47(3)	53(4)	-4(3)	8(3)	4(3)
C(51)	37(2)	39(3)	36(3)	-1(2)	2(2)	5(2)
C(52)	46(3)	50(3)	39(3)	-8(3)	6(2)	-6(2)
C(53)	50(3)	55(4)	56(4)	-2(3)	1(3)	-13(3)
C(54)	62(4)	55(4)	67(4)	-9(3)	-9(3)	-19(3)
C(55)	77(4)	59(4)	40(3)	-13(3)	-1(3)	-6(3)
C(56)	49(3)	51(3)	39(3)	-4(3)	1(2)	5(2)
C(61)	34(2)	44(3)	45(3)	6(2)	8(2)	4(2)
C(62)	49(3)	49(3)	50(3)	9(3)	1(3)	2(3)
C(63)	64(4)	57(4)	66(4)	21(3)	15(3)	-7(3)
C(64)	72(4)	60(4)	61(4)	25(3)	14(3)	2(3)
C(65)	66(4)	80(5)	55(4)	18(4)	-4(3)	6(4)
C(66)	49(3)	63(4)	49(3)	21(3)	5(3)	0(3)
C(70)	48(3)	50(3)	32(3)	-7(2)	4(2)	-6(2)
C(71)	44(3)	75(4)	37(3)	-1(3)	12(2)	-17(3)
C(72)	66(3)	45(3)	38(3)	13(2)	13(3)	-14(3)
C(73)	61(3)	46(3)	36(3)	2(2)	2(2)	-1(3)
C(74)	45(3)	60(3)	32(3)	12(3)	3(2)	-6(3)
C(75)	45(3)	60(3)	38(3)	-4(3)	-3(2)	1(2)
C(76)	60(4)	78(5)	49(4)	-15(3)	-12(3)	-11(3)
C(77)	84(5)	58(4)	56(4)	-17(3)	4(3)	-1(3)
C(78)	59(3)	77(4)	43(3)	-9(3)	4(3)	10(3)
C(1)	37(2)	37(3)	45(3)	3(2)	6(2)	-4(2)
C(2)	50(3)	45(3)	63(4)	5(3)	1(3)	-3(3)
C(3)	40(3)	48(3)	73(4)	11(3)	10(3)	-8(2)
C(81)	44(3)	70(5)	67(4)	5(3)	5(3)	-18(3)
C(82)	92(5)	91(6)	105(7)	-17(5)	43(5)	-36(5)
C(83)	148(10)	155(12)	157(12)	-67(10)	88(10)	-70(9)
C(84)	101(8)	273(22)	86(8)	-36(11)	19(6)	-82(12)
C(85)	62(5)	190(13)	96(8)	65(8)	-8(5)	-35(6)
C(86)	60(4)	99(6)	93(6)	33(5)	-4(4)	-18(4)
C(91)	41(3)	45(3)	73(4)	10(3)	2(3)	-7(2)
C(92)	52(3)	63(4)	96(5)	11(4)	15(4)	-10(3)
C(93)	81(5)	74(5)	94(6)	-9(4)	8(4)	-7(4)
C(94)	83(5)	79(5)	90(6)	3(5)	-18(4)	-26(4)
C(95)	64(4)	76(5)	84(5)	19(4)	-12(4)	-31(4)

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Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}]. (Cont.).

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{13}
C(96)	49(3)	70(4)	76(5)	21(4)	0(3)	-18(3)
P(3)	60(1)	69(1)	42(1)	5(1)	10(1)	5(1)
F(1)	146(4)	90(3)	79(3)	1(2)	61(3)	-12(3)
F(2)	117(4)	140(5)	103(4)	25(3)	-8(3)	41(3)
F(3)	199(5)	106(4)	67(3)	-23(3)	40(3)	-75(4)
F(4)	220(6)	78(3)	82(3)	-14(3)	59(4)	-10(3)
F(5)	148(4)	213(6)	89(3)	-43(4)	74(3)	-96(4)
F(6)	136(5)	304(10)	140(6)	24(6)	-20(4)	122(6)
C(900)	337(25)	353(26)	296(23)	249(21)	-183(19)	-282(22)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3).

	x	y	z	U_{iso}
H(12)	904(4)	1901(3)	2972(3)	75(3)
H(13)	-844(5)	1895(4)	2828(4)	75(3)
H(14)	-1782(4)	1528(4)	1840(4)	75(3)
H(15)	-954(4)	1231(4)	1009(4)	75(3)
H(16)	808(4)	1240(3)	1149(3)	75(3)
H(22)	2393(4)	626(3)	3117(3)	75(3)
H(23)	2706(6)	552(4)	4251(4)	75(3)
H(24)	3344(5)	1474(5)	4861(3)	75(3)
H(25)	3580(4)	2504(4)	4366(3)	75(3)
H(26)	3246(4)	2583(3)	3232(3)	75(3)
H(32)	4155(4)	2491(3)	2132(3)	75(3)
H(33)	4426(5)	3607(3)	1899(3)	75(3)
H(34)	3074(6)	4328(3)	1601(5)	75(3)
H(35)	1456(6)	3955(4)	1574(5)	75(3)
H(36)	1140(4)	2822(3)	1762(4)	75(3)
H(42)	6831(4)	519(3)	2299(3)	75(3)
H(43)	7842(5)	-237(4)	1839(4)	75(3)
H(44)	7136(6)	-1106(4)	1193(4)	75(3)
H(45)	5418(5)	-1289(3)	1045(3)	75(3)
H(46)	4375(5)	-568(3)	1504(3)	75(3)
H(52)	5937(4)	1503(3)	1692(3)	75(3)
H(53)	6766(4)	2519(3)	1941(3)	75(3)
H(54)	6742(4)	3021(3)	2942(3)	75(3)
H(55)	5809(5)	2555(3)	3660(3)	75(3)
H(56)	4982(4)	1532(3)	3416(3)	75(3)
H(62)	3291(4)	-399(3)	2642(3)	75(3)
H(63)	3247(5)	-1065(3)	3541(3)	75(3)
H(64)	4416(5)	-921(3)	4462(3)	75(3)
H(65)	5701(5)	-143(4)	4491(3)	75(3)
H(66)	5809(4)	509(3)	3576(3)	75(3)
H(71)	4848(4)	900(3)	858(2)	75(3)
H(72)	4131(4)	2055(3)	987(3)	75(3)
H(73)	2247(4)	1962(3)	717(2)	75(3)
H(75)	897(4)	907(3)	47(3)	75(3)
H(76)	926(5)	-176(3)	-359(3)	75(3)
H(77)	2408(5)	-792(3)	-249(3)	75(3)
H(78)	3915(5)	-339(3)	233(3)	75(3)
H(82)	554(6)	214(5)	2645(4)	75(3)
H(83)	266(9)	159(7)	3693(7)	75(3)
H(84)	508(9)	-808(9)	4268(6)	75(3)
H(85)	905(6)	-1790(7)	3798(5)	75(3)
H(86)	1093(5)	-1792(4)	2701(4)	75(3)
H(92)	1726(5)	-1291(3)	869(4)	75(3)
H(93)	1005(6)	-2100(4)	124(4)	75(3)
H(94)	-535(6)	-2576(4)	228(4)	75(3)
H(95)	-1381(5)	-2232(4)	1026(4)	75(3)
H(96)	-666(4)	-1442(3)	1787(3)	75(3)
H(99A)[1]	2567(12)	6295(7)	494(7)	208(53)
H(99B)[1]	1363(12)	6301(7)	359(7)	208(53)
H(99C)[2]	2174(12)	6339(7)	248(7)	208(53)
H(99D)[2]	2406(12)	6181(7)	1004(7)	208(53)

[1] Occupation factor = 0.57(1)
[2] Occupation factor = 0.43(1)

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Table 7. Torsion Angles [°].

C74	-Ru1	-C1	-C2	8.(2)	C73	-Ru1	-C1	-C2	33.(3)
C72	-Ru1	-C1	-C2	7.(3)	C71	-Ru1	-C1	-C2	-45.(3)
C70	-Ru1	-C1	-C2	-27.(2)	P2	-Ru1	-C1	-C2	-140.(2)
P1	-Ru1	-C1	-C2	123.(2)	C73	-Ru1	-C74	-C75	-128.1(7)
C72	-Ru1	-C74	-C75	-166.1(6)	C71	-Ru1	-C74	-C75	151.9(6)
C70	-Ru1	-C74	-C75	114.2(6)	P2	-Ru1	-C74	-C75	125.8(5)
P1	-Ru1	-C74	-C75	-76.9(5)	C1	-Ru1	-C74	-C70	-100.0(4)
C73	-Ru1	-C74	-C70	117.7(5)	C72	-Ru1	-C74	-C70	79.8(4)
C71	-Ru1	-C74	-C70	37.7(3)	P2	-Ru1	-C74	-C70	11.7(5)
P1	-Ru1	-C74	-C70	168.9(3)	C1	-Ru1	-C74	-C73	142.3(4)
C72	-Ru1	-C74	-C73	-37.9(3)	C71	-Ru1	-C74	-C73	-80.0(4)
C70	-Ru1	-C74	-C73	-117.7(5)	P2	-Ru1	-C74	-C73	-106.0(4)
P1	-Ru1	-C74	-C73	51.2(4)	C72	-Ru1	-C73	-C74	115.7(5)
C71	-Ru1	-C73	-C74	78.4(4)	C70	-Ru1	-C73	-C74	35.9(3)
P2	-Ru1	-C73	-C74	123.9(3)	P1	-Ru1	-C73	-C74	-135.1(3)
C1	-Ru1	-C73	-C72	-162.1(4)	C74	-Ru1	-C73	-C72	-115.7(5)
C71	-Ru1	-C73	-C72	-37.3(3)	C70	-Ru1	-C73	-C72	-79.8(4)
P2	-Ru1	-C73	-C72	8.2(5)	P1	-Ru1	-C73	-C72	109.2(3)
C71	-Ru1	-C72	-C73	116.8(5)	C70	-Ru1	-C72	-C73	78.4(4)
P2	-Ru1	-C72	-C73	-174.5(3)	P1	-Ru1	-C72	-C73	-74.5(3)
C1	-Ru1	-C72	-C71	-78.4(7)	C74	-Ru1	-C72	-C71	-78.9(4)
C73	-Ru1	-C72	-C71	-116.8(5)	C70	-Ru1	-C72	-C71	-38.4(3)
P2	-Ru1	-C72	-C71	68.6(3)	P1	-Ru1	-C72	-C71	168.7(3)
C70	-Ru1	-C71	-C72	115.3(5)	P2	-Ru1	-C71	-C72	-115.0(3)
P1	-Ru1	-C71	-C72	-16.3(5)	C1	-Ru1	-C71	-C70	30.8(5)
C74	-Ru1	-C71	-C70	-36.0(3)	C73	-Ru1	-C71	-C70	-78.0(4)
C72	-Ru1	-C71	-C70	-115.3(5)	P2	-Ru1	-C71	-C70	129.7(3)
P1	-Ru1	-C71	-C70	-131.6(3)	P2	-Ru1	-C70	-C71	-55.6(3)
P1	-Ru1	-C70	-C71	97.8(4)	P2	-Ru1	-C70	-C74	-173.0(3)
P1	-Ru1	-C70	-C74	-19.7(5)	P2	-Ru1	-C70	-C78	72.5(5)
P1	-Ru1	-C70	-C78	-134.2(5)	P1	-Ru1	-P2	-C41	-177.4(2)
P1	-Ru1	-P2	-C51	-61.1(2)	P1	-Ru1	-P2	-C61	65.6(3)
P2	-Ru1	-P1	-C31	102.5(2)	P2	-Ru1	-P1	-C21	-20.0(3)
P2	-Ru1	-P1	-C11	-141.9(2)	C70	-Ru1	-P1	-C31	-52.5(4)
C70	-Ru1	-P1	-C21	-175.1(4)	C70	-Ru1	-P1	-C11	63.1(4)
C71	-Ru1	-P1	-C31	7.1(4)	C71	-Ru1	-P1	-C21	-115.4(3)
C71	-Ru1	-P1	-C11	122.8(3)	C72	-Ru1	-P1	-C31	-2.6(3)
C72	-Ru1	-P1	-C21	-125.2(3)	C72	-Ru1	-P1	-C11	113.0(3)
C73	-Ru1	-P1	-C31	-37.4(3)	C73	-Ru1	-P1	-C21	-159.9(3)
C73	-Ru1	-P1	-C11	78.3(3)	C74	-Ru1	-P1	-C31	-64.8(3)
C74	-Ru1	-P1	-C21	172.6(3)	C74	-Ru1	-P1	-C11	50.8(3)
C1	-Ru1	-P1	-C31	-160.1(3)	C1	-Ru1	-P1	-C21	77.3(3)
C1	-Ru1	-P1	-C11	-44.5(3)	C70	-Ru1	-P2	-C61	-127.9(3)
C70	-Ru1	-P2	-C51	105.4(3)	C70	-Ru1	-P2	-C41	-10.9(3)
C71	-Ru1	-P2	-C61	-157.4(3)	C71	-Ru1	-P2	-C51	75.9(3)
C71	-Ru1	-P2	-C41	-40.5(3)	C72	-Ru1	-P2	-C61	169.2(3)
C72	-Ru1	-P2	-C51	42.5(3)	C72	-Ru1	-P2	-C41	-73.8(3)
C73	-Ru1	-P2	-C61	164.3(3)	C73	-Ru1	-P2	-C51	37.5(4)
C73	-Ru1	-P2	-C41	-78.8(4)	C74	-Ru1	-P2	-C61	-135.0(4)
C74	-Ru1	-P2	-C51	98.3(4)	C74	-Ru1	-P2	-C41	-18.1(4)
C1	-Ru1	-P2	-C61	-24.0(3)	C1	-Ru1	-P2	-C51	-150.7(3)
C1	-Ru1	-P2	-C41	93.0(3)	C71	-Ru1	-C70	-C78	128.1(7)
C71	-Ru1	-C70	-C74	-117.4(5)	C72	-Ru1	-C70	-C78	166.1(6)
C72	-Ru1	-C70	-C74	-79.4(4)	C72	-Ru1	-C70	-C71	38.0(3)
C73	-Ru1	-C70	-C78	-151.8(6)	C73	-Ru1	-C70	-C74	-37.3(3)
C73	-Ru1	-C70	-C71	80.1(4)	C74	-Ru1	-C70	-C78	-114.5(7)
C74	-Ru1	-C70	-C71	117.4(5)	C1	-Ru1	-C70	-C78	-29.6(6)
C1	-Ru1	-C70	-C74	84.9(4)	C1	-Ru1	-C70	-C71	-157.7(4)
C73	-Ru1	-C71	-C72	37.3(3)	C74	-Ru1	-C71	-C72	79.3(4)
C1	-Ru1	-C71	-C72	146.1(4)	C74	-Ru1	-C72	-C73	37.9(3)
C1	-Ru1	-C72	-C73	38.4(7)	C1	-Ru1	-C73	-C74	-46.4(4)
C1	-Ru1	-C74	-C75	14.2(5)	Ru1	-P1	-C31	-C32	-57.8(5)
Ru1	-P1	-C31	-C36	121.4(5)	Ru1	-P1	-C21	-C22	-59.0(5)
Ru1	-P1	-C21	-C26	123.2(5)	Ru1	-P1	-C11	-C12	156.2(4)
Ru1	-P1	-C11	-C16	-27.4(6)	C21	-P1	-C31	-C32	75.1(5)
C11	-P1	-C31	-C32	179.6(4)	C21	-P1	-C31	-C36	-105.8(5)
C11	-P1	-C31	-C36	-1.2(6)	C11	-P1	-C21	-C22	68.8(5)
C11	-P1	-C21	-C26	-109.0(5)	C21	-P1	-C11	-C16	-160.2(5)

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Table 7. Torsion Angles [°]. (Cont.).

C21	-P1	-C11	-C12	23.4(5)	C31	-P1	-C11	-C16	93.6(5)
C31	-P1	-C11	-C12	-82.7(5)	C31	-P1	-C21	-C26	-3.4(6)
C31	-P1	-C21	-C22	174.4(5)	Ru1	-P2	-C61	-C62	32.5(6)
Ru1	-P2	-C61	-C66	-154.4(4)	Ru1	-P2	-C51	-C52	-70.9(5)
Ru1	-P2	-C51	-C56	100.6(5)	Ru1	-P2	-C41	-C42	137.4(5)
Ru1	-P2	-C41	-C46	-46.8(5)	C51	-P2	-C61	-C62	161.3(5)
C41	-P2	-C61	-C62	-91.0(5)	C51	-P2	-C61	-C66	-25.6(6)
C41	-P2	-C61	-C66	82.1(5)	C41	-P2	-C51	-C52	50.3(5)
C41	-P2	-C51	-C56	-138.2(5)	C51	-P2	-C41	-C46	-167.2(5)
C51	-P2	-C41	-C42	17.0(6)	C61	-P2	-C41	-C46	83.4(5)
C61	-P2	-C41	-C42	-92.4(5)	C61	-P2	-C51	-C56	-34.5(5)
C61	-P2	-C51	-C52	154.0(4)	P1	-C11	-C16	-C15	-176.1(5)
P1	-C11	-C12	-C13	176.1(5)	C12	-C11	-C16	-C15	0.2(9)
C16	-C11	-C12	-C13	-0.3(9)	C11	-C12	-C13	-C14	1.(1)
C12	-C13	-C14	-C15	-2.(1)	C13	-C14	-C15	-C16	1.(1)
C14	-C15	-C16	-C11	-1.(1)	P1	-C21	-C26	-C25	177.1(5)
P1	-C21	-C22	-C23	-176.8(5)	C22	-C21	-C26	-C25	-0.7(9)
C26	-C21	-C22	-C23	1.1(9)	C21	-C22	-C23	-C24	-2.(1)
C22	-C23	-C24	-C25	2.(1)	C23	-C24	-C25	-C26	-2.(1)
C24	-C25	-C26	-C21	1.(1)	P1	-C31	-C36	-C35	178.7(6)
P1	-C31	-C32	-C33	179.9(5)	C32	-C31	-C36	-C35	-2.(1)
C36	-C31	-C32	-C33	0.7(9)	C31	-C32	-C33	-C34	0.(1)
C32	-C33	-C34	-C35	1.(1)	C33	-C34	-C35	-C36	-2.(1)
C34	-C35	-C36	-C31	3.(1)	P2	-C41	-C46	-C45	179.9(5)
P2	-C41	-C42	-C43	179.2(5)	C42	-C41	-C46	-C45	-4.2(9)
C46	-C41	-C42	-C43	3.5(9)	C41	-C42	-C43	-C44	0.(1)
C42	-C43	-C44	-C45	-2.(1)	C43	-C44	-C45	-C46	2.(1)
C44	-C45	-C46	-C41	1.(1)	P2	-C51	-C56	-C55	-172.9(5)
P2	-C51	-C52	-C53	173.4(5)	C52	-C51	-C56	-C55	-1.2(8)
C56	-C51	-C52	-C53	1.4(8)	C51	-C52	-C53	-C54	0.3(9)
C52	-C53	-C54	-C55	-2.(1)	C53	-C54	-C55	-C56	2.(1)
C54	-C55	-C56	-C51	-0.7(9)	P2	-C61	-C66	-C65	-176.8(5)
P2	-C61	-C62	-C63	175.6(5)	C62	-C61	-C66	-C65	-3.5(9)
C66	-C61	-C62	-C63	2.1(9)	C61	-C62	-C63	-C64	1.(1)
C62	-C63	-C64	-C65	-2.(1)	C63	-C64	-C65	-C66	0.(1)
C64	-C65	-C66	-C61	2.(1)	C71	-C70	-C74	-Ru1	-58.9(4)
Ru1	-C70	-C78	-C77	90.3(7)	Ru1	-C70	-C74	-C75	-123.4(5)
Ru1	-C70	-C74	-C73	58.4(4)	Ru1	-C70	-C71	-C72	-65.5(4)
C74	-C70	-C71	-Ru1	62.0(4)	C78	-C70	-C71	-Ru1	-119.8(7)
C78	-C70	-C74	-Ru1	122.6(6)	C74	-C70	-C78	-C77	0.8(9)
C71	-C70	-C78	-C77	-177.2(7)	C71	-C70	-C74	-C75	177.7(5)
C78	-C70	-C74	-C73	-178.9(5)	C71	-C70	-C74	-C73	-0.4(6)
C74	-C70	-C71	-C72	-3.5(7)	C78	-C70	-C71	-C72	174.7(6)
C78	-C70	-C74	-C75	-0.8(9)	C70	-C71	-C72	-Ru1	67.8(4)
C70	-C71	-C72	-C73	6.1(7)	Ru1	-C71	-C72	-C73	-61.8(4)
C71	-C72	-C73	-Ru1	62.3(4)	C71	-C72	-C73	-C74	-6.4(7)
Ru1	-C72	-C73	-C74	-68.7(4)	Ru1	-C73	-C74	-C70	-62.2(4)
C72	-C73	-C74	-C70	4.3(7)	C72	-C73	-C74	-Ru1	66.4(4)
C72	-C73	-C74	-C75	-173.5(6)	Ru1	-C73	-C74	-C75	120.1(7)
C73	-C74	-C75	-C76	177.3(6)	C70	-C74	-C75	-C76	-0.2(9)
Ru1	-C74	-C75	-C76	-90.2(7)	C74	-C75	-C76	-C77	1.(1)
C75	-C76	-C77	-C78	-1.(1)	C76	-C77	-C78	-C70	0.(1)
Ru1	-C1	-C2	-C3	-175.(2)	C1	-C2	-C3	-C81	16.(3)
C1	-C2	-C3	-C91	-164.(3)	C2	-C3	-C91	-C92	29.(1)
C2	-C3	-C91	-C96	-150.7(6)	C2	-C3	-C81	-C82	45.(1)
C2	-C3	-C81	-C86	-130.9(7)	C81	-C3	-C91	-C92	-150.6(6)
C81	-C3	-C91	-C96	29.7(9)	C91	-C3	-C81	-C86	48.7(9)
C91	-C3	-C81	-C82	-135.8(7)	C3	-C81	-C86	-C85	174.4(8)
C3	-C81	-C82	-C83	-176.7(9)	C82	-C81	-C86	-C85	-1.(1)
C86	-C81	-C82	-C83	-1.(1)	C81	-C82	-C83	-C84	3.(2)
C82	-C83	-C84	-C85	-3.(2)	C83	-C84	-C85	-C86	0.(2)
C84	-C85	-C86	-C81	2.(2)	C3	-C91	-C96	-C95	179.1(6)
C3	-C91	-C92	-C93	-179.7(7)	C92	-C91	-C96	-C95	-1.(1)
C96	-C91	-C92	-C93	0.(1)	C91	-C92	-C93	-C94	0.(1)
C92	-C93	-C94	-C95	1.(1)	C93	-C94	-C95	-C96	-2.(1)
C94	-C95	-C96	-C91	2.(1)	C11	-C900	-C12	-C12'	-100.0(9)
C11	-C900	-C12'	-C12	98.9(9)					

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Table 8. Torsion Angles [°] involving hydrogen atoms.

C72	-Ru1	-C73	-H73	-121.4(8)	C71	-Ru1	-C73	-H73	-158.7(7)
C70	-Ru1	-C73	-H73	158.8(7)	P2	-Ru1	-C73	-H73	-113.2(6)
P1	-Ru1	-C73	-H73	-12.2(6)	C71	-Ru1	-C72	-H72	-121.8(8)
C70	-Ru1	-C72	-H72	-160.3(8)	P2	-Ru1	-C72	-H72	-53.2(7)
P1	-Ru1	-C72	-H72	46.9(7)	C70	-Ru1	-C71	-H71	-123.2(8)
P2	-Ru1	-C71	-H71	6.6(6)	P1	-Ru1	-C71	-H71	105.3(6)
C72	-Ru1	-C71	-H71	121.6(8)	C73	-Ru1	-C71	-H71	158.9(7)
C74	-Ru1	-C71	-H71	-159.1(7)	C1	-Ru1	-C71	-H71	-92.3(7)
C73	-Ru1	-C72	-H72	121.3(8)	C74	-Ru1	-C72	-H72	159.3(8)
C1	-Ru1	-C72	-H72	159.8(7)	C74	-Ru1	-C73	-H73	122.9(8)
C1	-Ru1	-C73	-H73	76.5(7)	P1	-C11	-C16	-H16	4.(1)
P1	-C11	-C12	-H12	-4.(1)	C12	-C11	-C16	-H16	-179.8(8)
C16	-C11	-C12	-H12	179.6(8)	C11	-C12	-C13	-H13	-179.0(9)
H12	-C12	-C13	-H13	1.(1)	H12	-C12	-C13	-C14	-179.0(8)
C12	-C13	-C14	-H14	178.5(9)	H13	-C13	-C14	-H14	-2.(1)
H13	-C13	-C14	-C15	178.5(9)	C13	-C14	-C15	-H15	-178.6(9)
H14	-C14	-C15	-H15	1.(1)	H14	-C14	-C15	-C16	-178.6(9)
H15	-C15	-C16	-C11	179.2(9)	C14	-C15	-C16	-H16	179.2(8)
H15	-C15	-C16	-H16	-1.(1)	P1	-C21	-C26	-H26	-3.(1)
P1	-C21	-C22	-H22	3.(1)	C22	-C21	-C26	-H26	179.4(7)
C26	-C21	-C22	-H22	-178.9(7)	C21	-C22	-C23	-H23	178.2(9)
H22	-C22	-C23	-H23	-2.(1)	H22	-C22	-C23	-C24	178.2(8)
C22	-C23	-C24	-H24	-178.0(9)	H23	-C23	-C24	-H24	2.(2)
H23	-C23	-C24	-C25	-178.(1)	C23	-C24	-C25	-H25	178.5(9)
H24	-C24	-C25	-H25	-2.(1)	H24	-C24	-C25	-C26	178.5(9)
H25	-C25	-C26	-C21	-179.2(8)	C24	-C25	-C26	-H26	-179.2(8)
H25	-C25	-C26	-H26	1.(1)	P1	-C31	-C36	-H36	-1.(1)
P1	-C31	-C32	-H32	-0.1(9)	C32	-C31	-C36	-H36	177.9(8)
C36	-C31	-C32	-H32	-179.3(7)	C31	-C32	-C33	-H33	179.9(8)
H32	-C32	-C33	-H33	0.(1)	H32	-C32	-C33	-C34	179.9(8)
C32	-C33	-C34	-H34	-179.0(9)	H33	-C33	-C34	-H34	1.(1)
H33	-C33	-C34	-C35	-179.0(9)	C33	-C34	-C35	-H35	178.(1)
H34	-C34	-C35	-H35	-2.(2)	H34	-C34	-C35	-C36	178.(1)
H35	-C35	-C36	-C31	-177.(1)	C34	-C35	-C36	-H36	-177.0(9)
H35	-C35	-C36	-H36	3.(2)	P2	-C41	-C46	-H46	0.(1)
P2	-C41	-C42	-H42	-1.(1)	C42	-C41	-C46	-H46	175.8(8)
C46	-C41	-C42	-H42	-176.5(8)	C41	-C42	-C43	-H43	179.8(9)
H42	-C42	-C43	-H43	0.(1)	H42	-C42	-C43	-C44	179.8(9)
C42	-C43	-C44	-H44	177.5(9)	H43	-C43	-C44	-H44	-2.(2)
H43	-C43	-C44	-C45	177.5(9)	C43	-C44	-C45	-H45	-178.2(9)
H44	-C44	-C45	-H45	2.(1)	H44	-C44	-C45	-C46	-178.2(9)
H45	-C45	-C46	-C41	-178.5(8)	C44	-C45	-C46	-H46	-178.5(8)
H45	-C45	-C46	-H46	2.(1)	P2	-C51	-C56	-H56	7.1(9)
P2	-C51	-C52	-H52	-6.7(9)	C52	-C51	-C56	-H56	178.8(7)
C56	-C51	-C52	-H52	-178.6(7)	C51	-C52	-C53	-H53	-179.7(7)
H52	-C52	-C53	-H53	0.(1)	H52	-C52	-C53	-C54	-179.7(7)
C52	-C53	-C54	-H54	177.7(8)	H53	-C53	-C54	-H54	-2.(1)
H53	-C53	-C54	-C55	177.7(8)	C53	-C54	-C55	-H55	-177.5(8)
H54	-C54	-C55	-H55	2.(1)	H54	-C54	-C55	-C56	-177.5(8)
H55	-C55	-C56	-C51	179.3(8)	C54	-C55	-C56	-H56	179.3(7)
H55	-C55	-C56	-H56	-1.(1)	P2	-C61	-C66	-H66	3.(1)
P2	-C61	-C62	-H62	-4.4(9)	C62	-C61	-C66	-H66	176.5(7)
C66	-C61	-C62	-H62	-177.9(7)	C61	-C62	-C63	-H63	-179.5(8)
H62	-C62	-C63	-H63	1.(1)	H62	-C62	-C63	-C64	-179.5(8)
C62	-C63	-C64	-H64	178.2(8)	H63	-C63	-C64	-H64	-2.(1)
H63	-C63	-C64	-C65	178.2(8)	C63	-C64	-C65	-H65	-179.6(9)
H64	-C64	-C65	-H65	0.(1)	H64	-C64	-C65	-C66	-179.6(8)
H65	-C65	-C66	-C61	-177.7(8)	C64	-C65	-C66	-H66	-177.7(8)
H65	-C65	-C66	-H66	2.(1)	Ru1	-C70	-C78	-H78	-89.7(9)
Ru1	-C70	-C71	-H71	114.5(8)	C74	-C70	-C78	-H78	-179.2(8)
C71	-C70	-C78	-H78	3.(1)	C74	-C70	-C71	-H71	176.5(8)
C78	-C70	-C71	-H71	-5.(1)	H71	-C71	-C72	-Ru1	-112.2(8)
C70	-C71	-C72	-H72	-173.9(8)	Ru1	-C71	-C72	-H72	118.2(8)
H71	-C71	-C72	-H72	6.(1)	H71	-C71	-C72	-C73	-173.9(8)
H72	-C72	-C73	-Ru1	-117.7(8)	C71	-C72	-C73	-H73	173.6(8)
Ru1	-C72	-C73	-H73	111.3(8)	H72	-C72	-C73	-H73	-6.(1)
H72	-C72	-C73	-C74	173.6(8)	H73	-C73	-C74	-Ru1	-113.6(8)
H73	-C73	-C74	-C70	-175.8(7)	H73	-C73	-C74	-C75	6.(1)

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Table 8. Torsion Angles [°] involving hydrogen atoms. (Cont.).

C73	-C74	-C75	-H75	-3.(1)	C70	-C74	-C75	-H75	179.8(7)
Ru1	-C74	-C75	-H75	89.8(8)	C74	-C75	-C76	-H76	-178.8(8)
H75	-C75	-C76	-H76	1.(1)	H75	-C75	-C76	-C77	-178.8(8)
C75	-C76	-C77	-H77	178.8(8)	H76	-C76	-C77	-H77	-1.(1)
H76	-C76	-C77	-C78	178.8(8)	H77	-C77	-C78	-C70	-179.9(8)
C76	-C77	-C78	-H78	-179.9(8)	H77	-C77	-C78	-H78	0.(1)
C3	-C81	-C86	-H86	-6.(1)	C3	-C81	-C82	-H82	3.(1)
C82	-C81	-C86	-H86	179.(1)	C86	-C81	-C82	-H82	179.(1)
C81	-C82	-C83	-H83	-177.(1)	H82	-C82	-C83	-H83	3.(2)
H82	-C82	-C83	-C84	-177.(1)	C82	-C83	-C84	-H84	177.(2)
H83	-C83	-C84	-H84	-3.(3)	H83	-C83	-C84	-C85	177.(2)
C83	-C84	-C85	-H85	-180.(2)	H84	-C84	-C85	-H85	0.(3)
H84	-C84	-C85	-C86	-180.(2)	H85	-C85	-C86	-C81	-178.(1)
C84	-C85	-C86	-H86	-178.(1)	H85	-C85	-C86	-H86	2.(2)
C3	-C91	-C96	-H96	-1.(1)	C3	-C91	-C92	-H92	0.(1)
C92	-C91	-C96	-H96	179.4(8)	C96	-C91	-C92	-H92	180.0(8)
C91	-C92	-C93	-H93	179.7(9)	H92	-C92	-C93	-H93	0.(2)
H92	-C92	-C93	-C94	179.7(9)	C92	-C93	-C94	-H94	-179.(1)
H93	-C93	-C94	-H94	1.(2)	H93	-C93	-C94	-C95	-179.(1)
C93	-C94	-C95	-H95	178.(1)	H94	-C94	-C95	-H95	-2.(2)
H94	-C94	-C95	-C96	178.(1)	H95	-C95	-C96	-C91	-178.5(9)
C94	-C95	-C96	-H96	-178.5(9)	H95	-C95	-C96	-H96	2.(1)
C11	-C900	-C12	-H99D	110.(2)	C11	-C900	-C12'	-H99B	-109.(2)
C11	-C900	-H99D	-C12	-82.(2)	C11	-C900	-H99D	-H99A	107.(2)
C11	-C900	-H99C	-H99A	-99.(2)	C11	-C900	-H99C	-H99B	107.(2)
C11	-C900	-H99B	-H99C	-107.(2)	C11	-C900	-H99B	-C12'	83.(2)
C11	-C900	-H99A	-H99C	98.(2)	C11	-C900	-H99A	-H99D	-106.(2)
C12'	-C900	-C12	-H99D	-150.(2)	H99C	-C900	-C12	-H99D	-42.(3)
H99B	-C900	-C12	-H99D	-131.(2)	H99A	-C900	-C12	-H99D	-9.(2)
H99D	-C900	-C12	-C12'	150.(2)	H99C	-C900	-C12	-C12'	108.(3)
H99B	-C900	-C12	-C12'	19.(1)	H99A	-C900	-C12	-C12'	141.(2)
H99D	-C900	-C12'	-C12	-20.(1)	H99C	-C900	-C12'	-C12	-142.(2)
H99B	-C900	-C12'	-C12	-152.(2)	H99A	-C900	-C12'	-C12	-108.(3)
C12	-C900	-C12'	-H99B	152.(2)	H99D	-C900	-C12'	-H99B	132.(2)
H99C	-C900	-C12'	-H99B	10.(2)	H99A	-C900	-C12'	-H99B	44.(3)
H99C	-C900	-H99D	-C12	155.(2)	H99B	-C900	-H99D	-C12	71.(3)
H99A	-C900	-H99D	-C12	171.(2)	C12	-C900	-H99D	-H99A	-171.(2)
C12'	-C900	-H99D	-H99A	-140.(2)	H99C	-C900	-H99D	-H99A	-17.(2)
H99B	-C900	-H99D	-H99A	-100.(3)	C12	-C900	-H99C	-H99A	52.(3)
C12'	-C900	-H99C	-H99A	148.(2)	H99D	-C900	-H99C	-H99A	25.(2)
H99B	-C900	-H99C	-H99A	155.(2)	C12	-C900	-H99C	-H99B	-103.(3)
C12'	-C900	-H99C	-H99B	-7.(1)	H99D	-C900	-H99C	-H99B	-130.(2)
H99A	-C900	-H99C	-H99B	-155.(2)	H99A	-C900	-H99B	-H99C	17.(2)
H99A	-C900	-H99B	-C12'	-153.(2)	H99B	-C900	-H99A	-H99D	130.(2)
H99B	-C900	-H99A	-H99C	-26.(2)	H99C	-C900	-H99A	-H99D	155.(2)
H99D	-C900	-H99A	-H99C	-155.(2)	C12'	-C900	-H99A	-H99D	102.(3)
C12'	-C900	-H99A	-H99C	-54.(3)	C12	-C900	-H99A	-H99D	6.(1)
C12	-C900	-H99A	-H99C	-149.(2)	H99C	-C900	-H99B	-C12'	-170.(2)
H99D	-C900	-H99B	-C12'	-70.(3)	H99D	-C900	-H99B	-H99C	100.(3)
C12'	-C900	-H99B	-H99C	170.(2)	C12	-C900	-H99B	-C12'	-29.(2)
C12	-C900	-H99B	-H99C	141.(2)	C12'	-C900	-H99D	-C12	31.(2)
H99C	-H99A	-H99D	-C900	27.(2)	C900	-H99A	-H99D	-C12	-23.(5)
C900	-H99A	-H99C	-H99B	23.(2)	H99D	-H99A	-H99C	-C900	-23.(2)
H99C	-H99A	-H99D	-C12	3.(6)	H99D	-H99A	-H99C	-H99B	1.(3)
C900	-H99B	-H99C	-H99A	-27.(2)	H99C	-H99B	-C12'	-C900	-25.(5)
C900	-H99B	-C12'	-C12	21.(1)	C12'	-H99B	-H99C	-H99A	2.(7)
C12'	-H99B	-H99C	-C900	29.(5)	H99C	-H99B	-C12'	-C12	-3.(5)
H99A	-H99D	-C12	-C900	19.(4)	H99A	-H99D	-C12	-C12'	-4.(5)
C900	-H99D	-C12	-C12'	-24.(1)	C900	-C12'	-C12	-H99D	16.(1)
H99B	-C12'	-C12	-H99D	2.(1)	H99B	-C12'	-C12	-C900	-14.(1)

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Table 9. Slip parameter Δ[a] ,selected bond lengths [Å], selected angles, FA[a], HA[a], CA[a] and DA[a] [°].

Δ			0.121(5)
Ru	-C*		1.951(5)
C*	-Ru	-C1	124.1(2)
C*	-Ru	-P1	121.6(2)
C*	-Ru	-P2	120.6(2)
FA			8.1(3)
HA			6.2(4)
CA			9.6(3)
DA			164.5(3)

C* = Centroid (C70, C71, C72, C73, C74)
C** = Centroid (C70, C74, C75, C76, C77, C78)

[a] Δ = d [Ru - C74,C70] - d [Ru - C71,C73]
Fold angle (FA) = angle between normals to least-squares planes defined by C71, C72, C73 and C70, C74, C75, C76, C77, C78.
Hinge angle (HA) = angle between normals to least-squares planes defined by C71, C72, C73 and C71, C74, C70, C73.
Conformational angle (CA) = angle between normals to least-squares planes defined by C**, C*, Ru and C*, Ru, C1.
Dihedral angle (DA) = angle between normals to least-squares planes defined by C*, Ru, C1 and C1, C2, C3, C81, C91.

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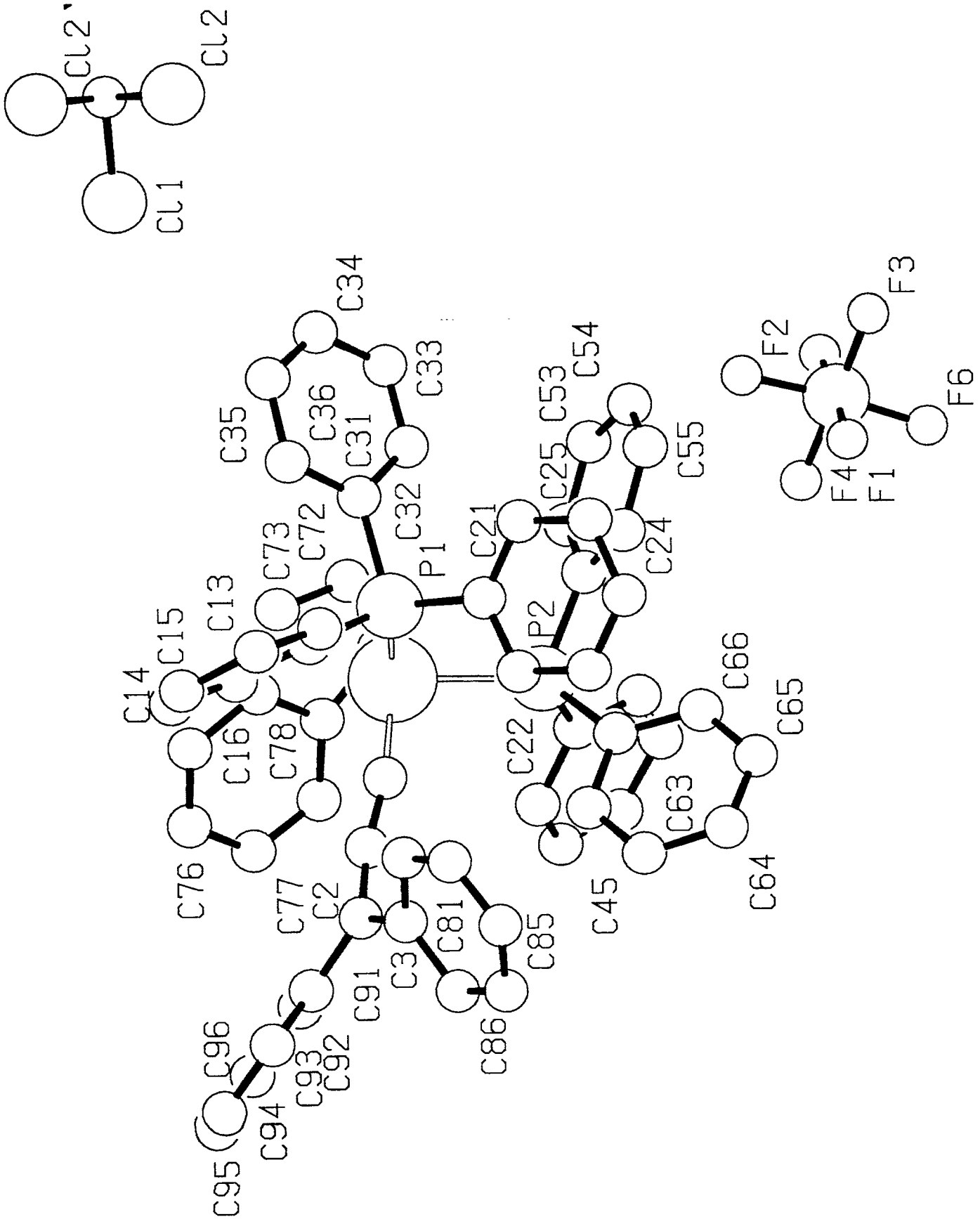
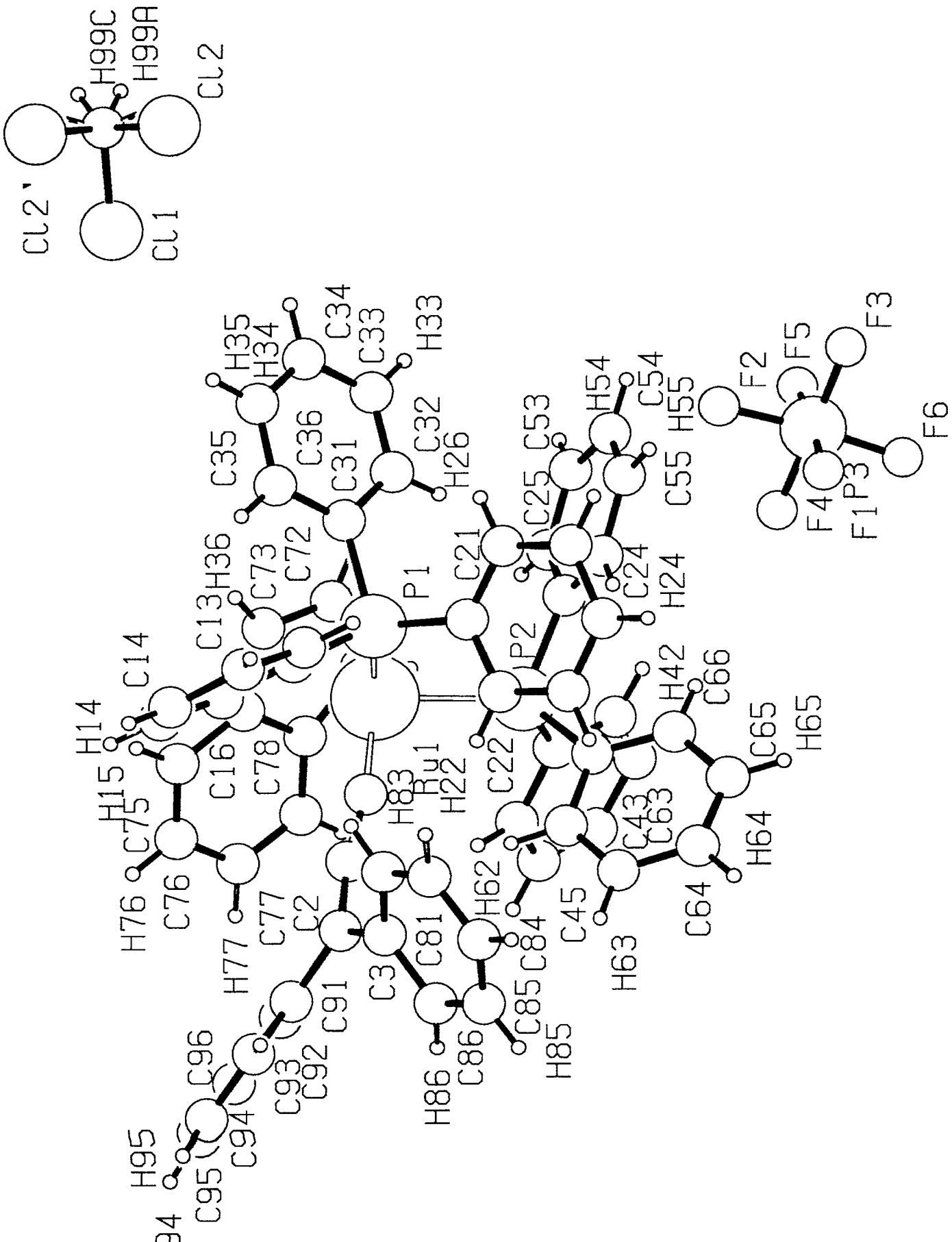


L214722


H99C
H99A
Cl2
Cl2'
Cl1
H35
H34
C34
C33
H33
C35
C36
C31
C32
H26
C53
H54
C54
H55
C55
F2
F5
F3
F6
F4
F1
P3
H36
C73
C72
P1
C21
C25
C24
H24
C13
C14
H14
H15
C75
C16
C78
H83
Ru1
H22
C22
P2
H42
C66
C65
H65
C76
H76
C77
H77
C2
C3
C81
H62
C84
C45
C43
C63
H64
C64
H63
C91
C92
C93
C94
C96
C95
H95
C86
H86
C85
H85

Compound 3m L2147-23

X-RAY DIFFRACTION STUDY

Data collection, crystal, and refinement parameters are collected in Table 1. The unit cell parameters were obtained from the least-squares fit of 25 reflections (with θ between 15° and 20°). Data were collected with the ω-2θ scan technique and a variable scan rate with a maximum scan time of 60 s per reflection. On all reflections, profile analysis[2,4] was performed. Lorentz and polarization corrections were applied and the data were reduced to $|F_o|$ values.

The structure was solved by DIRDIF[1] (Patterson methods and phases expansion). Isotropic least-squares refinement using SHELX76[6,9] converged to R = 0.088. At this stage an empirical absorption correction was applied using DIFABS[10].

Hydrogen atoms were geometrically placed. During the final stages of the refinement, the positional parameters and the anisotropic thermal parameters of the non-H atoms were refined. The hydrogen atoms were isotropically refined with a common thermal parameter, riding on their parent atoms.

Finally, a full-matrix least-squares refinement on F^2 was made using SHELXL93[7]. The function minimized was $w = 1/[\sigma^2(F_o^2)+(0.0671*P)^2]$ where $P = (Max(F_o^2,0)+2*F_c^2)/3$, with $\sigma^2(F_o^2)$ from counting statistics. The maximum shift to e.s.d. ratio in the last full-matrix least-squares cycle was 0.020. The CH_2Cl_2 solvent molecule which was affected of strong structural disorder was refined as a rigid group with its hydrogen atoms geometrically placed and refined with fixed (1.2 times the thermal parameter of the bonded carbon atom) thermal parameters. The final difference Fourier map showed no peaks higher than 1.52 $eÅ^{-3}$ near to the disordered CH_2Cl_2, nor deeper than -1.24 $eÅ^{-3}$. Atomic scattering factors were taken from International Tables for X-ray Crystallography (1974)[3]. Geometrical calculations were made with PARST[5]. The crystallographic plots were made with EUCLID[8]. All calculations were made at the University of Oviedo on the Scientific Computer Center and X-Ray group VAX-computers. This work was partially supported by DGICYT (PB93 - 0330). Javier Borge thanks to the Ministerio de Educación y Ciencia (Spain) for a fellowship.

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Table 1. Crystal data and structure refinement for OS21B.

Identification code	OS21B
Empirical formula	$C_{60}H_{47}F_6OsP_3 \cdot CH_2Cl_2$
Formula weight	1250.08 $gmol^{-1}$
Temperature	200 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 13.308(4) Å α = 90° b = 19.382(8) Å β = 100.47(7)° c = 20.735(14) Å γ = 90°
Volume	5259(4) $Å^3$
Z	4
Density (calculated)	1.579 Mgm^{-3}
Absorption coefficient	2.679 mm^{-1}
F(000)	2496
Crystal size	0.46 x 0.46 x 0.20 mm
θ range for data collection	1.45° to 24.99°
Index ranges	0<=h<=15, 0<=k<=23, -24<=l<=24
Reflections collected	9841
Independent reflections	9239 [R(int) = 0.034]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9239 / 0 / 659
Goodness-of-fit on F^2	1.048
Final R indices [I>2σ(I)]	R1 = 0.033, wR2 = 0.097
R indices (all data)	R1 = 0.045, wR2 = 0.098
Largest diff. peak and hole	1.52 and -1.24 $eÅ^{-3}$

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for OS21B. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Os	1830(1)	945(1)	3515(1)	23(1)
P(1)	2558(1)	1673(1)	2845(1)	25(1)
P(2)	374(1)	681(1)	2730(1)	24(1)
C(11)	2374(3)	2578(2)	3038(2)	32(1)
C(12)	3186(4)	3031(3)	3202(3)	56(2)
C(13)	3000(4)	3715(3)	3342(5)	85(3)
C(14)	2044(5)	3956(3)	3312(4)	65(2)
C(15)	1221(4)	3519(2)	3139(3)	45(1)
C(16)	1396(3)	2830(2)	2997(2)	35(1)
C(21)	2209(3)	1643(2)	1951(2)	31(1)
C(22)	2396(4)	1037(2)	1638(2)	38(1)
C(23)	2181(5)	987(3)	958(3)	52(1)
C(24)	1784(4)	1549(3)	590(3)	55(2)
C(25)	1611(4)	2162(3)	892(2)	49(1)
C(26)	1829(3)	2212(3)	1570(2)	38(1)
C(31)	3955(3)	1606(2)	2949(2)	28(1)
C(32)	4526(3)	1412(3)	3543(3)	43(1)
C(33)	5586(4)	1420(3)	3644(3)	53(1)
C(34)	6082(4)	1604(3)	3145(3)	53(1)
C(35)	5523(4)	1794(3)	2544(3)	50(1)
C(36)	4456(3)	1799(3)	2454(2)	39(1)
C(41)	-386(3)	1450(2)	2468(2)	25(1)
C(42)	-917(3)	1762(2)	2914(2)	28(1)
C(43)	-1411(3)	2390(2)	2765(2)	36(1)
C(44)	-1400(4)	2705(2)	2171(2)	40(1)
C(45)	-864(4)	2407(2)	1732(2)	40(1)
C(46)	-366(3)	1784(2)	1873(2)	32(1)
C(51)	-519(3)	113(2)	3065(2)	28(1)
C(52)	-1558(4)	206(3)	2945(3)	42(1)
C(53)	-2187(4)	-249(3)	3213(3)	54(1)
C(54)	-1778(4)	-795(3)	3580(3)	49(1)
C(55)	-739(5)	-901(2)	3692(3)	46(1)
C(56)	-114(4)	-456(2)	3427(2)	36(1)
C(61)	460(3)	191(2)	1981(2)	29(1)
C(62)	-273(4)	258(2)	1423(2)	37(1)
C(63)	-216(4)	-143(3)	874(2)	44(1)
C(64)	554(4)	-623(3)	883(2)	44(1)
C(65)	1266(4)	-703(3)	1447(2)	40(1)
C(66)	1226(3)	-303(2)	1992(2)	36(1)
C(70)	2559(4)	986(2)	4632(2)	31(1)
C(71)	2298(4)	1659(2)	4367(2)	33(1)
C(72)	1215(4)	1701(2)	4184(2)	35(1)
C(73)	814(4)	1050(2)	4275(2)	34(1)
C(74)	1629(3)	604(2)	4573(2)	32(1)
C(75)	1641(4)	-87(2)	4814(2)	38(1)
C(76)	2550(4)	-361(3)	5104(2)	47(1)
C(77)	3473(4)	28(3)	5178(2)	46(1)
C(78)	3494(3)	681(3)	4949(2)	36(1)
C(1)	2687(3)	221(2)	3322(2)	27(1)
C(2)	3310(4)	-269(2)	3308(2)	38(1)
C(3)	3950(4)	-760(3)	3159(3)	41(1)
C(81)	4178(4)	-749(3)	2486(3)	44(1)
C(82)	4454(5)	-145(3)	2212(4)	66(2)
C(83)	4594(6)	-129(5)	1572(4)	90(3)

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for OS21B. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor. (Cont.).

	x	y	z	U(eq)
C(84)	4473(6)	-701(6)	1201(4)	98(3)
C(85)	4189(5)	-1321(5)	1462(3)	77(2)
C(86)	4059(4)	-1344(3)	2099(3)	56(2)
C(91)	4387(4)	-1297(2)	3624(3)	40(1)
C(92)	3914(4)	-1514(3)	4122(3)	48(1)
C(93)	4344(4)	-2029(3)	4558(3)	58(2)
C(94)	5257(5)	-2320(3)	4492(3)	57(2)
C(95)	5754(4)	-2106(3)	4013(3)	56(2)
C(96)	5328(4)	-1598(3)	3565(3)	48(1)
P(3)	8611(1)	2435(1)	4752(1)	36(1)
F(1)	8945(3)	3072(2)	5229(2)	66(1)
F(2)	8301(3)	1793(2)	4275(2)	67(1)
F(3)	9352(3)	2696(2)	4283(2)	57(1)
F(4)	7889(3)	2172(2)	5225(2)	80(1)
F(5)	9510(3)	1996(2)	5156(2)	69(1)
F(6)	7724(3)	2888(3)	4345(2)	95(1)
C(900)	6948(10)	1115(6)	579(5)	133(4)
Cl(1)	6943(3)	217(2)	370(1)	158(1)
Cl(2)	6915(3)	1164(2)	1378(2)	163(1)

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Table 3. Bond lengths [Å] for OS21B.

Os-C(1)	1.895(4)
Os-C(71)	2.242(4)
Os-C(73)	2.265(5)
Os-C(72)	2.272(4)
Os-P(1)	2.312(2)
Os-C(70)	2.344(5)
Os-P(2)	2.350(2)
Os-C(74)	2.353(4)
P(1)-C(11)	1.826(4)
P(1)-C(21)	1.829(5)
P(1)-C(31)	1.838(4)
P(2)-C(41)	1.828(4)
P(2)-C(61)	1.842(4)
P(2)-C(51)	1.846(4)
C(11)-C(16)	1.378(6)
C(11)-C(12)	1.386(7)
C(12)-C(13)	1.389(8)
C(12)-H(12)	0.93
C(13)-C(14)	1.346(8)
C(13)-H(13)	0.93
C(14)-C(15)	1.380(7)
C(14)-H(14)	0.93
C(15)-C(16)	1.396(6)
C(15)-H(15)	0.93
C(16)-H(16)	0.93
C(21)-C(22)	1.385(6)
C(21)-C(26)	1.397(6)
C(22)-C(23)	1.390(7)
C(22)-H(22)	0.93
C(23)-C(24)	1.379(8)
C(23)-H(23)	0.93
C(24)-C(25)	1.382(8)
C(24)-H(24)	0.93
C(25)-C(26)	1.387(7)
C(25)-H(25)	0.93
C(26)-H(26)	0.93
C(31)-C(36)	1.373(6)
C(31)-C(32)	1.377(6)
C(32)-C(33)	1.388(7)
C(32)-H(32)	0.93
C(33)-C(34)	1.371(8)
C(33)-H(33)	0.93
C(34)-C(35)	1.382(8)
C(34)-H(34)	0.93
C(35)-C(36)	1.397(7)
C(35)-H(35)	0.93
C(36)-H(36)	0.93
C(41)-C(46)	1.398(6)
C(41)-C(42)	1.401(6)
C(42)-C(43)	1.391(6)
C(42)-H(42)	0.93
C(43)-C(44)	1.376(7)
C(43)-H(43)	0.93
C(44)-C(45)	1.382(7)
C(44)-H(44)	0.93
C(45)-C(46)	1.383(6)
C(45)-H(45)	0.93
C(46)-H(46)	0.93
C(51)-C(52)	1.371(6)
C(51)-C(56)	1.386(6)

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Table 3. Bond lengths [Å] for OS21B. (Cont.).

C(52)-C(53)	1.399(7)
C(52)-H(52)	0.93
C(53)-C(54)	1.359(8)
C(53)-H(53)	0.93
C(54)-C(55)	1.375(8)
C(54)-H(54)	0.93
C(55)-C(56)	1.381(7)
C(55)-H(55)	0.93
C(56)-H(56)	0.93
C(61)-C(62)	1.378(6)
C(61)-C(66)	1.395(6)
C(62)-C(63)	1.392(6)
C(62)-H(62)	0.93
C(63)-C(64)	1.382(7)
C(63)-H(63)	0.93
C(64)-C(65)	1.373(7)
C(64)-H(64)	0.93
C(65)-C(66)	1.380(7)
C(65)-H(65)	0.93
C(66)-H(66)	0.93
C(70)-C(74)	1.428(6)
C(70)-C(78)	1.426(6)
C(70)-C(71)	1.433(6)
C(71)-C(72)	1.424(6)
C(71)-H(71)	0.93
C(72)-C(73)	1.397(7)
C(72)-H(72)	0.93
C(73)-C(74)	1.436(6)
C(73)-H(73)	0.93
C(74)-C(75)	1.429(7)
C(75)-C(76)	1.357(7)
C(75)-H(75)	0.93
C(76)-C(77)	1.424(7)
C(76)-H(76)	0.93
C(77)-C(78)	1.353(7)
C(77)-H(77)	0.93
C(78)-H(78)	0.93
C(1)-C(2)	1.265(6)
C(2)-C(3)	1.349(7)
C(3)-C(91)	1.465(7)
C(3)-C(81)	1.482(8)
C(81)-C(82)	1.382(8)
C(81)-C(86)	1.396(8)
C(82)-C(83)	1.372(10)
C(82)-H(82)	0.93
C(83)-C(84)	1.341(13)
C(83)-H(83)	0.93
C(84)-C(85)	1.399(13)
C(84)-H(84)	0.93
C(85)-C(86)	1.364(9)
C(85)-H(85)	0.93
C(86)-H(86)	0.93
C(91)-C(92)	1.369(8)
C(91)-C(96)	1.407(7)
C(92)-C(93)	1.398(8)
C(92)-H(92)	0.93
C(93)-C(94)	1.369(8)
C(93)-H(93)	0.93
C(94)-C(95)	1.355(9)
C(94)-H(94)	0.93

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Table 3. Bond lengths [Å] for OS21B. (Cont.).

C(95)-C(96)	1.401(8)
C(95)-H(95)	0.93
C(96)-H(96)	0.93
P(3)-F(4)	1.578(3)
P(3)-F(5)	1.579(3)
P(3)-F(6)	1.585(4)
P(3)-F(3)	1.589(3)
P(3)-F(1)	1.594(3)
P(3)-F(2)	1.597(4)
C(900)-Cl(2)	1.670(10)
C(900)-Cl(1)	1.792(11)
C(900)-H(901)	0.97
C(900)-H(902)	0.97

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Table 4. Bond angles [°] for OS21B.

C(1)-Os-C(71)	122.1(2)
C(1)-Os-C(73)	132.2(2)
C(71)-Os-C(73)	60.7(2)
C(1)-Os-C(72)	154.7(2)
C(71)-Os-C(72)	36.8(2)
C(73)-Os-C(72)	35.9(2)
C(1)-Os-P(1)	89.51(14)
C(71)-Os-P(1)	90.58(13)
C(73)-Os-P(1)	136.99(12)
C(72)-Os-P(1)	102.09(14)
C(1)-Os-C(70)	94.4(2)
C(71)-Os-C(70)	36.3(2)
C(73)-Os-C(70)	60.1(2)
C(72)-Os-C(70)	60.3(2)
P(1)-Os-C(70)	115.43(12)
C(1)-Os-P(2)	98.36(13)
C(71)-Os-P(2)	139.12(12)
C(73)-Os-P(2)	88.81(13)
C(72)-Os-P(2)	102.70(12)
P(1)-Os-P(2)	95.73(5)
C(70)-Os-P(2)	146.38(12)
C(1)-Os-C(74)	99.4(2)
C(71)-Os-C(74)	60.0(2)
C(73)-Os-C(74)	36.2(2)
C(72)-Os-C(74)	59.8(2)
P(1)-Os-C(74)	149.58(12)
C(70)-Os-C(74)	35.4(2)
P(2)-Os-C(74)	111.43(12)
C(11)-P(1)-C(21)	103.5(2)
C(11)-P(1)-C(31)	102.4(2)
C(21)-P(1)-C(31)	100.4(2)
C(11)-P(1)-Os	111.6(2)
C(21)-P(1)-Os	122.18(14)
C(31)-P(1)-Os	114.30(14)
C(41)-P(2)-C(61)	106.6(2)
C(41)-P(2)-C(51)	103.9(2)
C(61)-P(2)-C(51)	98.8(2)
C(41)-P(2)-Os	111.73(14)
C(61)-P(2)-Os	121.7(2)
C(51)-P(2)-Os	112.07(14)
C(16)-C(11)-C(12)	118.4(4)
C(16)-C(11)-P(1)	119.3(3)
C(12)-C(11)-P(1)	122.2(4)
C(11)-C(12)-C(13)	119.7(5)
C(11)-C(12)-H(12)	120.2(3)
C(13)-C(12)-H(12)	120.2(3)
C(14)-C(13)-C(12)	121.7(5)
C(14)-C(13)-H(13)	119.2(3)
C(12)-C(13)-H(13)	119.2(3)
C(13)-C(14)-C(15)	119.9(5)
C(13)-C(14)-H(14)	120.1(3)
C(15)-C(14)-H(14)	120.1(3)
C(14)-C(15)-C(16)	119.1(5)
C(14)-C(15)-H(15)	120.4(3)
C(16)-C(15)-H(15)	120.4(3)
C(11)-C(16)-C(15)	121.2(4)
C(11)-C(16)-H(16)	119.4(3)
C(15)-C(16)-H(16)	119.4(3)
C(22)-C(21)-C(26)	118.9(4)

Table 4. Bond angles [°] for OS21B. (Cont.).

C(22)-C(21)-P(1)	117.9(3)
C(26)-C(21)-P(1)	123.1(4)
C(21)-C(22)-C(23)	120.8(5)
C(21)-C(22)-H(22)	119.6(3)
C(23)-C(22)-H(22)	119.6(3)
C(24)-C(23)-C(22)	119.6(5)
C(24)-C(23)-H(23)	120.2(3)
C(22)-C(23)-H(23)	120.2(3)
C(23)-C(24)-C(25)	120.5(5)
C(23)-C(24)-H(24)	119.7(3)
C(25)-C(24)-H(24)	119.7(3)
C(24)-C(25)-C(26)	119.9(5)
C(24)-C(25)-H(25)	120.1(3)
C(26)-C(25)-H(25)	120.1(3)
C(25)-C(26)-C(21)	120.3(5)
C(25)-C(26)-H(26)	119.8(3)
C(21)-C(26)-H(26)	119.8(3)
C(36)-C(31)-C(32)	118.6(4)
C(36)-C(31)-P(1)	120.8(3)
C(32)-C(31)-P(1)	120.4(3)
C(31)-C(32)-C(33)	120.8(5)
C(31)-C(32)-H(32)	119.6(3)
C(33)-C(32)-H(32)	119.6(3)
C(34)-C(33)-C(32)	120.3(5)
C(34)-C(33)-H(33)	119.9(3)
C(32)-C(33)-H(33)	119.9(3)
C(33)-C(34)-C(35)	119.7(5)
C(33)-C(34)-H(34)	120.2(3)
C(35)-C(34)-H(34)	120.2(3)
C(34)-C(35)-C(36)	119.4(5)
C(34)-C(35)-H(35)	120.3(3)
C(36)-C(35)-H(35)	120.3(3)
C(31)-C(36)-C(35)	121.2(5)
C(31)-C(36)-H(36)	119.4(3)
C(35)-C(36)-H(36)	119.4(3)
C(46)-C(41)-C(42)	118.5(4)
C(46)-C(41)-P(2)	122.8(3)
C(42)-C(41)-P(2)	118.3(3)
C(43)-C(42)-C(41)	120.3(4)
C(43)-C(42)-H(42)	119.8(3)
C(41)-C(42)-H(42)	119.8(2)
C(44)-C(43)-C(42)	120.4(4)
C(44)-C(43)-H(43)	119.8(3)
C(42)-C(43)-H(43)	119.8(3)
C(43)-C(44)-C(45)	119.7(4)
C(43)-C(44)-H(44)	120.2(3)
C(45)-C(44)-H(44)	120.2(3)
C(44)-C(45)-C(46)	120.7(4)
C(44)-C(45)-H(45)	119.7(3)
C(46)-C(45)-H(45)	119.7(3)
C(45)-C(46)-C(41)	120.4(4)
C(45)-C(46)-H(46)	119.8(3)
C(41)-C(46)-H(46)	119.8(3)
C(52)-C(51)-C(56)	118.9(4)
C(52)-C(51)-P(2)	123.3(3)
C(56)-C(51)-P(2)	117.6(3)
C(51)-C(52)-C(53)	120.1(5)
C(51)-C(52)-H(52)	120.0(3)
C(53)-C(52)-H(52)	120.0(3)
C(54)-C(53)-C(52)	120.4(5)

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Table 4. Bond angles [°] for OS21B. (Cont.).

C(54)-C(53)-H(53)	119.8(3)
C(52)-C(53)-H(53)	119.8(3)
C(53)-C(54)-C(55)	120.0(5)
C(53)-C(54)-H(54)	120.0(3)
C(55)-C(54)-H(54)	120.0(3)
C(54)-C(55)-C(56)	119.9(5)
C(54)-C(55)-H(55)	120.0(3)
C(56)-C(55)-H(55)	120.0(3)
C(55)-C(56)-C(51)	120.6(5)
C(55)-C(56)-H(56)	119.7(3)
C(51)-C(56)-H(56)	119.7(3)
C(62)-C(61)-C(66)	118.8(4)
C(62)-C(61)-P(2)	121.0(3)
C(66)-C(61)-P(2)	119.9(3)
C(61)-C(62)-C(63)	119.9(4)
C(61)-C(62)-H(62)	120.1(3)
C(63)-C(62)-H(62)	120.1(3)
C(64)-C(63)-C(62)	121.0(5)
C(64)-C(63)-H(63)	119.5(3)
C(62)-C(63)-H(63)	119.5(3)
C(65)-C(64)-C(63)	118.9(4)
C(65)-C(64)-H(64)	120.6(3)
C(63)-C(64)-H(64)	120.6(3)
C(64)-C(65)-C(66)	120.7(5)
C(64)-C(65)-H(65)	119.7(3)
C(66)-C(65)-H(65)	119.7(3)
C(65)-C(66)-C(61)	120.7(4)
C(65)-C(66)-H(66)	119.7(3)
C(61)-C(66)-H(66)	119.7(3)
C(74)-C(70)-C(78)	119.6(4)
C(74)-C(70)-C(71)	107.0(4)
C(78)-C(70)-C(71)	133.2(4)
C(74)-C(70)-Os	72.7(2)
C(78)-C(70)-Os	127.7(3)
C(71)-C(70)-Os	68.0(2)
C(72)-C(71)-C(70)	108.6(4)
C(72)-C(71)-Os	72.7(2)
C(70)-C(71)-Os	75.7(2)
C(72)-C(71)-H(71)	125.7(3)
C(70)-C(71)-H(71)	125.7(3)
Os-C(71)-H(71)	117.76(13)
C(73)-C(72)-C(71)	107.7(4)
C(73)-C(72)-Os	71.8(3)
C(71)-C(72)-Os	70.5(2)
C(73)-C(72)-H(72)	126.1(3)
C(71)-C(72)-H(72)	126.1(3)
Os-C(72)-H(72)	123.25(12)
C(72)-C(73)-C(74)	108.9(4)
C(72)-C(73)-Os	72.3(3)
C(74)-C(73)-Os	75.3(2)
C(72)-C(73)-H(73)	125.5(3)
C(74)-C(73)-H(73)	125.5(3)
Os-C(73)-H(73)	118.66(13)
C(70)-C(74)-C(75)	120.1(4)
C(70)-C(74)-C(73)	107.5(4)
C(75)-C(74)-C(73)	132.4(4)
C(70)-C(74)-Os	71.9(2)
C(75)-C(74)-Os	126.4(3)
C(73)-C(74)-Os	68.5(2)
C(76)-C(75)-C(74)	118.2(5)

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Table 4. Bond angles [°] for OS21B. (Cont.).

C(76)-C(75)-H(75)	120.9(3)
C(74)-C(75)-H(75)	120.9(3)
C(75)-C(76)-C(77)	121.5(5)
C(75)-C(76)-H(76)	119.3(3)
C(77)-C(76)-H(76)	119.3(3)
C(78)-C(77)-C(76)	122.0(5)
C(78)-C(77)-H(77)	119.0(3)
C(76)-C(77)-H(77)	119.0(3)
C(77)-C(78)-C(70)	118.5(5)
C(77)-C(78)-H(78)	120.8(3)
C(70)-C(78)-H(78)	120.8(3)
C(2)-C(1)-Os	169.3(4)
C(1)-C(2)-C(3)	168.0(5)
C(2)-C(3)-C(91)	122.8(5)
C(2)-C(3)-C(81)	116.8(5)
C(91)-C(3)-C(81)	120.4(4)
C(82)-C(81)-C(86)	118.3(6)
C(82)-C(81)-C(3)	121.0(5)
C(86)-C(81)-C(3)	120.6(5)
C(83)-C(82)-C(81)	120.6(7)
C(83)-C(82)-H(82)	119.7(5)
C(81)-C(82)-H(82)	119.7(4)
C(84)-C(83)-C(82)	120.8(8)
C(84)-C(83)-H(83)	119.6(5)
C(82)-C(83)-H(83)	119.6(5)
C(83)-C(84)-C(85)	120.1(7)
C(83)-C(84)-H(84)	120.0(5)
C(85)-C(84)-H(84)	120.0(5)
C(86)-C(85)-C(84)	119.5(7)
C(86)-C(85)-H(85)	120.3(5)
C(84)-C(85)-H(85)	120.3(5)
C(85)-C(86)-C(81)	120.6(7)
C(85)-C(86)-H(86)	119.7(5)
C(81)-C(86)-H(86)	119.7(4)
C(92)-C(91)-C(96)	118.5(5)
C(92)-C(91)-C(3)	122.2(4)
C(96)-C(91)-C(3)	119.3(5)
C(91)-C(92)-C(93)	121.2(5)
C(91)-C(92)-H(92)	119.4(3)
C(93)-C(92)-H(92)	119.4(3)
C(94)-C(93)-C(92)	119.7(6)
C(94)-C(93)-H(93)	120.1(4)
C(92)-C(93)-H(93)	120.1(3)
C(95)-C(94)-C(93)	120.5(5)
C(95)-C(94)-H(94)	119.8(3)
C(93)-C(94)-H(94)	119.8(4)
C(94)-C(95)-C(96)	120.6(5)
C(94)-C(95)-H(95)	119.7(3)
C(96)-C(95)-H(95)	119.7(3)
C(91)-C(96)-C(95)	119.5(5)
C(91)-C(96)-H(96)	120.3(3)
C(95)-C(96)-H(96)	120.3(3)
F(4)-P(3)-F(5)	89.1(2)
F(4)-P(3)-F(6)	91.8(2)
F(5)-P(3)-F(6)	178.8(3)
F(4)-P(3)-F(3)	179.2(2)
F(5)-P(3)-F(3)	90.1(2)
F(6)-P(3)-F(3)	89.0(2)
F(4)-P(3)-F(1)	89.8(2)
F(5)-P(3)-F(1)	89.4(2)

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Table 4. Bond angles [°] for OS21B. (Cont.).

F(6)-P(3)-F(1)	89.9(2)
F(3)-P(3)-F(1)	89.9(2)
F(4)-P(3)-F(2)	90.9(2)
F(5)-P(3)-F(2)	89.7(2)
F(6)-P(3)-F(2)	91.1(2)
F(3)-P(3)-F(2)	89.3(2)
F(1)-P(3)-F(2)	178.8(2)
Cl(2)-C(900)-Cl(1)	107.1(5)
Cl(2)-C(900)-H(901)	110.3(4)
Cl(1)-C(900)-H(901)	110.3(5)
Cl(2)-C(900)-H(902)	110.3(5)
Cl(1)-C(900)-H(902)	110.3(4)
H(901)-C(900)-H(902)	108.5

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Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3) for OS21B. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}]

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os	23(1)	22(1)	23(1)	0(1)	4(1)	3(1)
P(1)	23(1)	23(1)	29(1)	3(1)	4(1)	2(1)
P(2)	23(1)	24(1)	25(1)	0(1)	6(1)	1(1)
C(11)	35(2)	21(2)	39(2)	1(2)	6(2)	1(2)
C(12)	31(3)	35(3)	101(5)	-5(3)	6(3)	4(2)
C(13)	39(3)	33(3)	176(8)	-21(4)	4(4)	-11(2)
C(14)	50(3)	27(3)	117(6)	-15(3)	10(4)	2(2)
C(15)	39(3)	35(3)	59(3)	-3(2)	5(2)	10(2)
C(16)	32(2)	30(2)	39(2)	-1(2)	1(2)	0(2)
C(21)	25(2)	37(2)	31(2)	5(2)	6(2)	-3(2)
C(22)	36(3)	38(3)	38(3)	1(2)	5(2)	-3(2)
C(23)	60(4)	57(4)	38(3)	-11(2)	13(3)	-12(3)
C(24)	52(3)	85(4)	29(3)	8(3)	6(2)	-12(3)
C(25)	41(3)	69(4)	37(3)	18(3)	7(2)	1(3)
C(26)	34(2)	45(3)	36(2)	14(2)	9(2)	2(2)
C(31)	26(2)	23(2)	37(2)	1(2)	8(2)	0(2)
C(32)	27(2)	52(3)	49(3)	12(2)	2(2)	0(2)
C(33)	32(3)	59(3)	64(4)	21(3)	-2(2)	-1(2)
C(34)	24(2)	50(3)	83(4)	9(3)	7(3)	-2(2)
C(35)	33(3)	56(3)	66(4)	9(3)	23(3)	-4(2)
C(36)	32(2)	43(3)	41(3)	4(2)	8(2)	-5(2)
C(41)	23(2)	26(2)	25(2)	0(2)	1(2)	-1(2)
C(42)	29(2)	30(2)	25(2)	2(2)	3(2)	3(2)
C(43)	36(2)	34(2)	38(2)	-2(2)	7(2)	9(2)
C(44)	44(3)	31(2)	43(3)	4(2)	-1(2)	8(2)
C(45)	47(3)	39(3)	29(2)	8(2)	-2(2)	-1(2)
C(46)	30(2)	37(2)	28(2)	2(2)	3(2)	-3(2)
C(51)	30(2)	27(2)	28(2)	-2(2)	7(2)	-4(2)
C(52)	34(2)	37(3)	56(3)	7(2)	9(2)	-1(2)
C(53)	37(3)	49(3)	79(4)	3(3)	22(3)	-9(2)
C(54)	52(3)	43(3)	57(3)	4(3)	22(3)	-15(2)
C(55)	60(3)	31(3)	46(3)	6(2)	9(3)	-8(2)
C(56)	37(2)	35(2)	36(2)	1(2)	5(2)	0(2)
C(61)	29(2)	27(2)	31(2)	-3(2)	9(2)	-7(2)
C(62)	34(2)	41(3)	34(2)	-10(2)	4(2)	-1(2)
C(63)	49(3)	45(3)	34(3)	-10(2)	-2(2)	0(2)
C(64)	59(3)	40(3)	38(3)	-17(2)	19(2)	-5(2)
C(65)	40(3)	35(2)	47(3)	-10(2)	13(2)	1(2)
C(66)	33(2)	35(2)	38(3)	-6(2)	4(2)	-1(2)
C(70)	36(2)	35(2)	21(2)	-1(2)	2(2)	2(2)
C(71)	43(3)	31(2)	24(2)	-9(2)	3(2)	-1(2)
C(72)	43(3)	42(3)	22(2)	-6(2)	8(2)	16(2)
C(73)	29(2)	46(3)	30(2)	0(2)	11(2)	7(2)
C(74)	36(2)	45(3)	17(2)	-1(2)	6(2)	0(2)
C(75)	41(3)	44(3)	29(2)	7(2)	6(2)	-4(2)
C(76)	57(3)	39(3)	42(3)	12(2)	4(2)	1(2)
C(77)	47(3)	50(3)	35(3)	11(2)	-7(2)	9(2)
C(78)	30(2)	45(3)	31(2)	3(2)	0(2)	-1(2)
C(1)	28(2)	28(2)	24(2)	-2(2)	4(2)	5(2)
C(2)	35(2)	31(2)	46(3)	-5(2)	0(2)	5(2)
C(3)	29(2)	38(2)	53(3)	-11(2)	0(2)	3(2)
C(81)	31(2)	47(3)	51(3)	-4(2)	3(2)	15(2)
C(82)	64(4)	55(4)	86(5)	6(3)	33(4)	17(3)
C(83)	85(5)	98(6)	98(6)	36(5)	44(5)	44(5)

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Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3) for OS21B. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a^{*2} U_{11} + ... + 2 h k a* b* U_{12}]. (Cont.).

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(84)	70(5)	174(10)	52(4)	23(6)	13(4)	55(6)
C(85)	41(3)	123(7)	60(4)	-37(4)	-8(3)	19(4)
C(86)	40(3)	67(4)	58(4)	-21(3)	2(3)	7(3)
C(91)	32(2)	34(2)	51(3)	-9(2)	0(2)	5(2)
C(92)	32(3)	45(3)	66(4)	-3(3)	5(2)	6(2)
C(93)	54(3)	54(3)	62(4)	5(3)	3(3)	3(3)
C(94)	62(4)	43(3)	59(4)	0(3)	-8(3)	17(3)
C(95)	46(3)	60(3)	55(3)	-17(3)	-7(3)	29(3)
C(96)	36(3)	52(3)	55(3)	-17(3)	1(2)	14(2)
P(3)	37(1)	45(1)	27(1)	4(1)	7(1)	4(1)
F(1)	106(3)	50(2)	49(2)	-9(2)	29(2)	-9(2)
F(2)	88(3)	76(2)	39(2)	-12(2)	15(2)	-36(2)
F(3)	71(2)	56(2)	52(2)	3(2)	32(2)	-6(2)
F(4)	77(2)	116(3)	57(2)	-14(2)	40(2)	-42(2)
F(5)	75(2)	70(2)	54(2)	11(2)	-9(2)	22(2)
F(6)	67(2)	137(4)	76(3)	25(3)	0(2)	52(3)
C(900)	190(12)	119(8)	81(6)	28(6)	5(7)	-48(8)
Cl(1)	193(3)	172(3)	94(2)	-20(2)	-12(2)	87(3)
Cl(2)	143(3)	219(4)	132(3)	-46(3)	40(2)	-6(3)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for OS21B.

	x	y	z	U(eq)
H(12)	3852(4)	2878(3)	3218(3)	53(2)
H(13)	3549(4)	4014(3)	3458(5)	53(2)
H(14)	1939(5)	4416(3)	3409(4)	53(2)
H(15)	558(4)	3682(2)	3117(3)	53(2)
H(16)	843(3)	2536(2)	2873(2)	53(2)
H(22)	2669(4)	659(2)	1886(2)	53(2)
H(23)	2305(5)	577(3)	753(3)	53(2)
H(24)	1632(4)	1515(3)	135(3)	53(2)
H(25)	1348(4)	2540(3)	641(2)	53(2)
H(26)	1721(3)	2627(3)	1773(2)	53(2)
H(32)	4197(3)	1274(3)	3880(3)	53(2)
H(33)	5961(4)	1300(3)	4052(3)	53(2)
H(34)	6793(4)	1600(3)	3212(3)	53(2)
H(35)	5852(4)	1917(3)	2202(3)	53(2)
H(36)	4079(3)	1936(3)	2052(2)	53(2)
H(42)	-941(3)	1548(2)	3313(2)	53(2)
H(43)	-1750(3)	2599(2)	3068(2)	53(2)
H(44)	-1751(4)	3117(2)	2067(2)	53(2)
H(45)	-838(4)	2628(2)	1337(2)	53(2)
H(46)	-16(3)	1586(2)	1570(2)	53(2)
H(52)	-1844(4)	571(3)	2684(3)	53(2)
H(53)	-2890(4)	-176(3)	3141(3)	53(2)
H(54)	-2200(4)	-1098(3)	3755(3)	53(2)
H(55)	-458(5)	-1273(2)	3947(3)	53(2)
H(56)	586(4)	-538(2)	3492(2)	53(2)
H(62)	-805(4)	572(2)	1413(2)	53(2)
H(63)	-704(4)	-87(3)	495(2)	53(2)
H(64)	590(4)	-887(3)	513(2)	53(2)
H(65)	1780(4)	-1030(3)	1461(2)	53(2)
H(66)	1714(3)	-362(2)	2369(2)	53(2)
H(71)	2758(4)	2009(2)	4323(2)	53(2)
H(72)	842(4)	2093(2)	4032(2)	53(2)
H(73)	130(4)	925(2)	4160(2)	53(2)
H(75)	1042(4)	-343(2)	4773(2)	53(2)
H(76)	2572(4)	-812(3)	5257(2)	53(2)
H(77)	4078(4)	-172(3)	5390(2)	53(2)
H(78)	4105(3)	925(3)	4998(2)	53(2)
H(82)	4546(5)	256(3)	2463(4)	53(2)
H(83)	4774(6)	283(5)	1394(4)	53(2)
H(84)	4579(6)	-684(6)	770(4)	53(2)
H(85)	4089(5)	-1716(5)	1203(3)	53(2)
H(86)	3890(4)	-1759(3)	2278(3)	53(2)
H(92)	3296(4)	-1316(3)	4170(3)	53(2)
H(93)	4011(4)	-2173(3)	4892(3)	53(2)
H(94)	5538(5)	-2668(3)	4778(3)	53(2)
H(95)	6384(4)	-2297(3)	3981(3)	53(2)
H(96)	5664(4)	-1460(3)	3230(3)	53(2)
H(901)	7560(10)	1336(6)	486(5)	159
H(902)	6357(10)	1344(6)	325(5)	159

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Table 7. Torsion Angles (°) for OS21B.

C73	-Os	-C74	-C75	127.6(6)	C72	-Os	-C74	-C75	165.2(5)
C71	-Os	-C74	-C75	-152.0(5)	C70	-Os	-C74	-C75	-114.6(6)
P2	-Os	-C74	-C75	72.6(5)	P1	-Os	-C74	-C75	-135.7(4)
C1	-Os	-C74	-C70	84.3(3)	C73	-Os	-C74	-C70	-117.9(4)
C72	-Os	-C74	-C70	-80.2(3)	C71	-Os	-C74	-C70	-37.5(3)
P2	-Os	-C74	-C70	-172.8(3)	P1	-Os	-C74	-C70	-21.1(5)
C1	-Os	-C74	-C73	-157.9(3)	C72	-Os	-C74	-C73	37.6(3)
C71	-Os	-C74	-C73	80.4(3)	C70	-Os	-C74	-C73	117.9(4)
P2	-Os	-C74	-C73	-54.9(3)	P1	-Os	-C74	-C73	96.7(4)
C72	-Os	-C73	-C74	-115.8(4)	C71	-Os	-C73	-C74	-78.2(3)
C70	-Os	-C73	-C74	-36.2(3)	P2	-Os	-C73	-C74	130.4(3)
P1	-Os	-C73	-C74	-132.5(3)	C1	-Os	-C73	-C72	145.9(3)
C74	-Os	-C73	-C72	115.8(4)	C71	-Os	-C73	-C72	37.6(3)
C70	-Os	-C73	-C72	79.6(3)	P2	-Os	-C73	-C72	-113.8(3)
P1	-Os	-C73	-C72	-16.7(4)	C71	-Os	-C72	-C73	-117.2(4)
C70	-Os	-C72	-C73	-79.0(3)	P2	-Os	-C72	-C73	69.6(3)
P1	-Os	-C72	-C73	168.4(3)	C1	-Os	-C72	-C71	41.2(6)
C74	-Os	-C72	-C71	79.2(3)	C73	-Os	-C72	-C71	117.2(4)
C70	-Os	-C72	-C71	38.2(3)	P2	-Os	-C72	-C71	-173.2(3)
P1	-Os	-C72	-C71	-74.4(3)	C70	-Os	-C71	-C72	-115.0(4)
P2	-Os	-C71	-C72	10.2(4)	P1	-Os	-C71	-C72	109.7(3)
C1	-Os	-C71	-C70	-45.5(4)	C74	-Os	-C71	-C70	36.5(3)
C73	-Os	-C71	-C70	78.3(3)	C72	-Os	-C71	-C70	115.0(4)
P2	-Os	-C71	-C70	125.2(3)	P1	-Os	-C71	-C70	-135.3(3)
P2	-Os	-C70	-C71	-105.1(4)	P1	-Os	-C70	-C71	51.1(3)
P2	-Os	-C70	-C74	12.1(5)	P1	-Os	-C70	-C74	168.3(3)
P2	-Os	-C70	-C78	126.6(4)	P1	-Os	-C70	-C78	-77.2(5)
P1	-Os	-P2	-C41	-61.2(2)	P1	-Os	-P2	-C51	-177.3(2)
P1	-Os	-P2	-C61	66.2(2)	P2	-Os	-P1	-C31	-142.0(2)
P2	-Os	-P1	-C21	-20.7(2)	P2	-Os	-P1	-C11	102.3(2)
C70	-Os	-P1	-C31	51.0(3)	C70	-Os	-P1	-C21	172.3(3)
C70	-Os	-P1	-C11	-64.7(3)	C71	-Os	-P1	-C31	78.5(2)
C71	-Os	-P1	-C21	-160.3(3)	C71	-Os	-P1	-C11	-37.2(2)
C72	-Os	-P1	-C31	113.7(2)	C72	-Os	-P1	-C21	-125.1(3)
C72	-Os	-P1	-C11	-2.0(3)	C73	-Os	-P1	-C31	123.6(3)
C73	-Os	-P1	-C21	-115.1(3)	C73	-Os	-P1	-C11	7.9(3)
C74	-Os	-P1	-C31	64.3(4)	C74	-Os	-P1	-C21	-174.4(3)
C74	-Os	-P1	-C11	-51.3(4)	C1	-Os	-P1	-C31	-43.7(3)
C1	-Os	-P1	-C21	77.6(3)	C1	-Os	-P1	-C11	-159.3(2)
C70	-Os	-P2	-C61	-135.3(3)	C70	-Os	-P2	-C51	-18.8(4)
C70	-Os	-P2	-C41	97.3(3)	C71	-Os	-P2	-C61	163.8(3)
C71	-Os	-P2	-C51	-79.8(3)	C71	-Os	-P2	-C41	36.3(3)
C72	-Os	-P2	-C61	170.0(3)	C72	-Os	-P2	-C51	-73.6(2)
C72	-Os	-P2	-C41	42.5(2)	C73	-Os	-P2	-C61	-156.7(3)
C73	-Os	-P2	-C51	-40.2(2)	C73	-Os	-P2	-C41	75.9(2)
C74	-Os	-P2	-C61	-127.8(3)	C74	-Os	-P2	-C51	-11.3(3)
C74	-Os	-P2	-C41	104.8(2)	C1	-Os	-P2	-C61	-24.1(3)
C1	-Os	-P2	-C51	92.3(3)	C1	-Os	-P2	-C41	-151.6(2)
C71	-Os	-C70	-C78	-128.4(6)	C71	-Os	-C70	-C74	117.2(4)
C72	-Os	-C70	-C78	-167.0(5)	C72	-Os	-C70	-C74	78.6(3)
C72	-Os	-C70	-C71	-38.6(3)	C73	-Os	-C70	-C78	151.4(5)
C73	-Os	-C70	-C74	37.0(3)	C73	-Os	-C70	-C71	-80.2(3)
C74	-Os	-C70	-C78	114.4(6)	C74	-Os	-C70	-C71	-117.2(4)
C1	-Os	-C70	-C78	14.3(5)	C1	-Os	-C70	-C74	-100.1(3)
C1	-Os	-C70	-C71	142.7(3)	C73	-Os	-C71	-C72	-36.7(3)
C74	-Os	-C71	-C72	-78.5(3)	C1	-Os	-C71	-C72	-160.6(3)
C74	-Os	-C72	-C73	-37.9(3)	C1	-Os	-C72	-C73	-76.0(6)
C1	-Os	-C73	-C74	30.1(4)	C1	-Os	-C74	-C75	-30.3(5)
Os	-P1	-C31	-C32	-28.7(5)	Os	-P1	-C31	-C36	156.4(4)
Os	-P1	-C21	-C22	-61.7(5)	Os	-P1	-C21	-C26	122.6(4)

Table 7. Torsion Angles (°) for OS21B. (Cont.)

Os	-P1	-C11	-C12	123.7(4)	Os	-P1	-C11	-C16	-58.8(5)
C21	-P1	-C31	-C32	-161.4(4)	C11	-P1	-C31	-C32	92.1(5)
C21	-P1	-C31	-C36	23.8(5)	C11	-P1	-C31	-C36	-82.7(5)
C11	-P1	-C21	-C22	171.6(4)	C11	-P1	-C21	-C26	-4.1(5)
C21	-P1	-C11	-C16	74.4(5)	C21	-P1	-C11	-C12	-103.2(5)
C31	-P1	-C11	-C16	178.5(4)	C31	-P1	-C11	-C12	1.0(5)
C31	-P1	-C21	-C26	-109.8(5)	C31	-P1	-C21	-C22	65.9(4)
Os	-P2	-C61	-C62	-154.7(4)	Os	-P2	-C61	-C66	31.0(5)
Os	-P2	-C51	-C52	137.3(4)	Os	-P2	-C51	-C56	-46.3(4)
Os	-P2	-C41	-C42	-70.4(4)	Os	-P2	-C41	-C46	102.2(4)
C51	-P2	-C61	-C62	82.4(5)	C41	-P2	-C61	-C62	-25.1(5)
C51	-P2	-C61	-C66	-91.8(4)	C41	-P2	-C61	-C66	160.7(4)
C41	-P2	-C51	-C52	16.5(5)	C41	-P2	-C51	-C56	-167.1(4)
C51	-P2	-C41	-C46	-136.9(4)	C51	-P2	-C41	-C42	50.6(4)
C61	-P2	-C41	-C46	-33.0(5)	C61	-P2	-C41	-C42	154.4(4)
C61	-P2	-C51	-C56	83.2(4)	C61	-P2	-C51	-C52	-93.1(5)
P1	-C11	-C16	-C15	-179.9(4)	P1	-C11	-C12	-C13	179.8(5)
C12	-C11	-C16	-C15	-2.2(8)	C16	-C11	-C12	-C13	2.2(9)
C11	-C12	-C13	-C14	-1.(1)	C12	-C13	-C14	-C15	0.(1)
C13	-C14	-C15	-C16	0.(1)	C14	-C15	-C16	-C11	1.1(8)
P1	-C21	-C26	-C25	177.8(4)	P1	-C21	-C22	-C23	-177.8(4)
C22	-C21	-C26	-C25	2.2(8)	C26	-C21	-C22	-C23	-1.9(8)
C21	-C22	-C23	-C24	0.5(9)	C22	-C23	-C24	-C25	0.8(9)
C23	-C24	-C25	-C26	-0.5(9)	C24	-C25	-C26	-C21	-1.0(9)
P1	-C31	-C36	-C35	175.6(4)	P1	-C31	-C32	-C33	-174.1(4)
C32	-C31	-C36	-C35	0.7(8)	C36	-C31	-C32	-C33	0.9(8)
C31	-C32	-C33	-C34	-1.8(9)	C32	-C33	-C34	-C35	1.2(9)
C33	-C34	-C35	-C36	0.3(9)	C34	-C35	-C36	-C31	-1.3(9)
P2	-C41	-C46	-C45	-172.6(4)	P2	-C41	-C42	-C43	172.8(4)
C42	-C41	-C46	-C45	-0.1(7)	C46	-C41	-C42	-C43	-0.1(7)
C41	-C42	-C43	-C44	1.3(7)	C42	-C43	-C44	-C45	-2.3(8)
C43	-C44	-C45	-C46	2.1(8)	C44	-C45	-C46	-C41	-0.9(8)
P2	-C51	-C56	-C55	180.0(4)	P2	-C51	-C52	-C53	179.6(4)
C52	-C51	-C56	-C55	-3.5(8)	C56	-C51	-C52	-C53	3.4(8)
C51	-C52	-C53	-C54	-1.9(9)	C52	-C53	-C54	-C55	0.5(9)
C53	-C54	-C55	-C56	-0.6(9)	C54	-C55	-C56	-C51	2.2(8)
P2	-C61	-C66	-C65	176.1(4)	P2	-C61	-C62	-C63	-176.9(4)
C62	-C61	-C66	-C65	1.8(8)	C66	-C61	-C62	-C63	-2.6(8)
C61	-C62	-C63	-C64	1.5(8)	C62	-C63	-C64	-C65	0.4(8)
C63	-C64	-C65	-C66	-1.3(8)	C64	-C65	-C66	-C61	0.1(8)
C71	-C70	-C74	-Os	59.6(3)	Os	-C70	-C78	-C77	-89.3(6)
Os	-C70	-C74	-C75	122.1(5)	Os	-C70	-C74	-C73	-59.6(4)
Os	-C70	-C71	-C72	65.9(4)	C74	-C70	-C71	-Os	-62.6(4)
C78	-C70	-C71	-Os	121.7(6)	C78	-C70	-C74	-Os	-124.0(5)
C74	-C70	-C78	-C77	1.1(7)	C71	-C70	-C78	-C77	176.3(6)
C71	-C70	-C74	-C75	-178.3(5)	C78	-C70	-C74	-C73	176.4(5)
C71	-C70	-C74	-C73	0.0(6)	C74	-C70	-C71	-C72	3.3(6)
C78	-C70	-C71	-C72	-172.4(5)	C78	-C70	-C74	-C75	-1.9(7)
C70	-C71	-C72	-Os	-67.8(4)	C70	-C71	-C72	-C73	-5.3(6)
Os	-C71	-C72	-C73	62.5(4)	C71	-C72	-C73	-Os	-61.7(4)
C71	-C72	-C73	-C74	5.3(6)	Os	-C72	-C73	-C74	67.0(4)
Os	-C73	-C74	-C70	61.8(4)	C72	-C73	-C74	-C70	-3.3(6)
C72	-C73	-C74	-Os	-65.1(4)	C72	-C73	-C74	-C75	174.7(5)
Os	-C73	-C74	-C75	-120.2(6)	C73	-C74	-C75	-C76	-176.9(6)
C70	-C74	-C75	-C76	0.9(8)	Os	-C74	-C75	-C76	89.9(6)
C74	-C75	-C76	-C77	0.9(8)	C75	-C76	-C77	-C78	-1.8(9)
C76	-C77	-C78	-C70	0.8(8)	C1	-C2	-C3	-C81	7.(3)
C1	-C2	-C3	-C91	-171.(2)	C2	-C3	-C91	-C92	26.0(9)
C2	-C3	-C91	-C96	-153.4(6)	C2	-C3	-C81	-C82	48.1(8)
C2	-C3	-C81	-C86	-128.0(6)	C81	-C3	-C91	-C92	-152.2(6)